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Implicit Runge–Kutta Methods with Explicit Internal Stages

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Abstract—The main computational costs of implicit Runge–Kutta methods are caused by solving a system of algebraic equations at every step. By introducing explicit stages, it is possible to increase the stage (or pseudo-stage) order of the method, which makes it possible to increase the accuracy and avoid reducing the order in solving stiff problems, without additional costs of solving algebraic equations. The paper presents implicit methods with an explicit first stage and one or two explicit internal stages. The results of solving test problems are compared with similar methods having no explicit internal stages.

Keywords: implicit Runge–Kutta methods, stiff problems, differential-algebraic problems, order reduction, stage order, pseudo-stage order.

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1. INTRODUCTION

One step of the numerical solution of a system of ordinary differential equations (ODEs)

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

by the Runge–Kutta method is defined by the formulas

$$\mathbf{y}_1 = \mathbf{y}_0 + h\sum_{i=1}^{s} b_i \mathbf{F}_i, \quad \mathbf{F}_i = \mathbf{f}(t_0 + c_i h, \mathbf{Y}_i), \quad \mathbf{Y}_i = \mathbf{y}_0 + h\sum_{j=1}^{s} a_{ij}\mathbf{F}_j, \quad i = 1,\ldots,s.$$

The convenience of the method can be conveniently represented by a Butcher table,

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

The matrix $\mathbf{A}$ of a fully implicit method has a full rank. In this case, the implementation of one step is reduced to a numerical solution of a system of nonlinear algebraic equations the size of which is equal to the product of the number of stages s by the number of equations in the system of ODEs. There are also implicit methods with an explicit first stage, the Butcher table of which has the form

$$\begin{array}{c|cc} 0 & 0 & \mathbf{0} \\ \tilde{\mathbf{c}} & \mathbf{a} & \tilde{\mathbf{A}} \\ \hline & b_1 & \tilde{\mathbf{b}}^{\mathrm{T}} \end{array}, \tag{1.1}$$

where the matrix $\tilde{\mathbf{A}}$ has a full rank. These include the Lobatto IIIA methods [1, 2], the diagonally implicit ESDIRK methods [3, 4], and the SAFERK methods considered in [5].

Denote by r the degree of the denominator of the stability function, calculated by formula

$$R(z) = \left|\mathbf{I} - z\mathbf{A} + z\mathbf{e}\mathbf{b}^{\mathrm{T}}\right| \Big/ \left|\mathbf{I} - z\mathbf{A}\right|, \quad \mathbf{e} = [1,\ldots,1]^{\mathrm{T}}, \quad \mathbf{I} = \mathrm{diag}(\mathbf{e}).$$

Suppose that the rank of the matrix $\mathbf{A}$ (or $\tilde{\mathbf{A}}$, for the method with an explicit first stage) is equal to r (this assumption holds for all methods considered in this paper). Then, among the rows of the matrix $\mathbf{A}$ (or $\tilde{\mathbf{A}}$) one can select r basis rows, through which the remaining rows are linearly expressed. The stages corresponding to the basis rows are considered implicit, and the remaining stages, explicit. The separation of stages into explicit and implicit is rather arbitrary, since the choice of basis rows is not unique. The values of explicit stages are linear combinations of the values of implicit stages; therefore, a system of algebraic equations can be formed and solved with respect to only implicit stages. Thus, the introduction of explicit stages makes it possible, with the same total number of stages, to reduce the size of the algebraic system to be solved.

Until recently, efficient implicit methods with explicit internal stages were not known. The Lobatto IIIB methods include an explicit internal stage, but they are not suitable for solving stiff problems (see [1]). Originally, efficient implicit methods with explicit first and explicit internal stages, called "implicit nested Gauss-type methods", were proposed in [6, 7] (see also [8, 9]). In [10], methods inverse to explicit methods, containing explicit internal stages and suitable for solving stiff problems and differential-algebraic problems of indices 2 and 3 were considered.

To understand why it is necessary to introduce explicit stages into an implicit method, let us consider methods of the sixth order with a stability function

$$R(z) = \frac{1 + z/2 + z^2/10 + z^3/120}{1 - z/2 + z^2/10 - z^3/120}.$$

Such are the three-stage Gauss method (Gauss63), the four-stage Lobatto IIIA method (Lobatto64), the seven-stage Kulikov method from [7–9] (Kulikov634), and the six-step IERK65 method (Implicit with Explicit stages Runge-Kutta). In the designation of the method, the first digit is the order p, the second digit is the stage order q, and the third digit is the pseudo-stage order $\overline{q}$ (present if $\overline{q} > q$). The definition of the pseudo-stage order is given in the next section. These methods were used for solving the problem

$$\begin{aligned} y_1' &= -(\mu + 2)y_1 + \mu y_2^2, \quad y_1(0) = 1, \\ y_2' &= y_1 - y_2 - y_2^2, \quad y_2(0) = 1, \quad 0 \le t \le 1, \end{aligned} \tag{1.2}$$

with the known exact solution $y_1(t) = \exp(-2t)$, $y_2(t) = \exp(-t)$, which is independent of the index of stiffness μ. Figure 1 shows the dependence of the errors of the solution and estimates of the order on the stiffness of the problem. The errors were calculated by the formula

$$e(h) = \max\left(\sqrt{e_1(t)^2 + e_2(t)^2}, 0 \le t \le 1\right), \tag{1.3}$$

where $e_i(t)$ is the error in the ith component with the step size $h = 1/10$, and the order estimates are calculated by the formula

$$\tilde{p} = \frac{\lg\left(e(h_1)/e(h_2)\right)}{\lg\left(h_1/h_2\right)}, \tag{1.4}$$

where $h_1 = 1/8$ and $h_2 = 1/12$.

The Gauss63 method does not contain explicit stages and is not stiffly accurate; therefore, it demonstrates the worst results. The introduction of an explicit first stage in the Lobatto64 method made it possible to increase the stage order to four and to make the method stiffly accurate, which led to a noticeable increase in accuracy. The Kulikov634 method has an explicit first and three implicit internal stages. The stage order of this method is only three, but it has the fourth pseudo-stage order; therefore, the error of this method behaves similarly to the error of the Lobatto64 method. However, the Kulikov634 method is mono-implicit, which gives some advantages (see [7–9]), but the Lobatto64 method is not. The IERK65 method has three explicit stages (the first and two internal ones), which made it possible to provide the fifth stage order and improve the accuracy in comparison with all other methods. Thus, the introduction of explicit stages made it possible to increase the stage (or pseudo-stage) order of the method, which led to a noticeable increase in accuracy.

The stage order of the Runge–Kutta method is defined as the largest integer number q for which

$$\mathbf{c}^k = k\mathbf{A}\mathbf{c}^{k-1}, \quad \mathbf{b}^{\mathrm{T}}\mathbf{c}^{k-1} = 1/k, \quad k = 1,\ldots,q \tag{1.5}$$

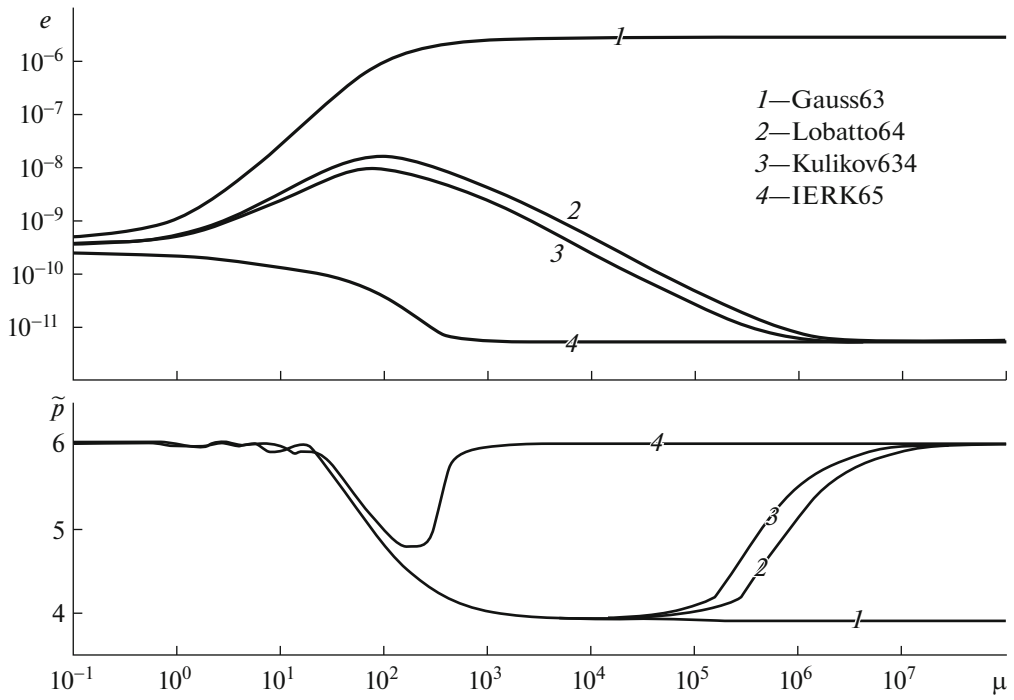

Fig. 1.

(hereinafter, we assume the component-wise execution of the vectors operations). The importance of a high stage order in solving stiff problems was noted in many works (see, e.g., [1, 2, 10, 11]). The large difference between the classical order p and the stage order q leads to a reduction in the actual order. To avoid a reduction in the order or make it insignificant, it is desirable that $q = p$ or $q = p - 1$.

For a given number of stages s, the maximum stage order $q = s$ is inherent in the collocation methods. For all other methods, $q < s$. For a given number of implicit stages r, the maximum order of a method is limited by the order of the consistency with the exponential of the stability function. For A-stable methods, the maximal order is $2r$ (as in the Gauss, Lobatto IIIA, and Lobatto IIIB methods, see [1, 2]) and, for L-stable methods, it is $2r - 1$ (as in the Radau IA and Radau IIA methods, see [1, 2]).

The implicit high-order methods used in practice, such as Radau IIA and Lobatto IIIA, have a large difference between the classical and stage orders, which can lead to a reduction in the actual order in solving stiff problems. For a given classical order, it is possible to increase the stage order by increasing the number of stages. However, if these stages are implicit, the computational costs of solving the algebraic system significantly increase. The introduction of explicit stages helps to avoid a noticeable increase in computational costs.

In this paper, we consider implicit methods of orders 3 to 6, containing an explicit first and one or two explicit internal stages. The results of the comparison with the Radau IIA and Lobatto IIIA methods, which have the same orders and stability functions but do not contain explicit internal stages, are presented.

2. PSEUDO-STAGE ORDER

The pseudo-stage order has the same significance as the stage order: its increase makes it possible to avoid a reduction in the actual order in solving stiff problems (see [10, 11]). At the same time, it does not have such restrictions as the stage order; the pseudo-stage order of explicit methods and inverse of them can be higher than 1, of diagonal-implicit methods, higher than 2; and, of the mono-implicit methods, higher than 3, as in the Kulikov634 method.

In [10, 11], the pseudo-stage order was defined in terms of the error functions $e_{ij}(z)$ proposed in [12]: a method has a pseudo-stage order $\overline{q}$ if all functions $e_{ij}(z)$ of orders $i \le \overline{q}$ are identically zero. Analytical expressions of the dependence of the error functions on the free parameters of the method can be very

Table 1

i	T_{ij}	Graph	$\gamma(T_{ij})$	$\boldsymbol{\Phi}(T_{ij})$
1	T_1		1	$\mathbf{e}$
2	T_{21}		2	$\mathbf{c}$
3	T_{31}		3	$\mathbf{c}^2$
	T_{32}		6	$\mathbf{Ac}$
4	T_{41}		4	$\mathbf{c}^3$
	T_{42}		8	$\mathbf{c(Ac)}$
	T_{43}		12	$\mathbf{Ac}^2$
	T_{44}		24	$\mathbf{A}^2\mathbf{c}$

cumbersome, which makes it difficult to use them when constructing new methods. Therefore, in this paper, an equivalent definition is given, which makes it possible to simplify the construction of methods of a given pseudo-stage order. For this, it is convenient to use some notation adopted in the conditions for the classical order.

The derivation of the conditions for the order of the Runge–Kutta methods is based on a one-to-one correspondence between elementary differentials and root trees (see [13]). As in [13], we will solve an autonomous system $\mathbf{y}' = \mathbf{f}(\mathbf{y})$. Define $\mathbf{c} = \mathbf{Ae}$, $\mathbf{e} = [1, \ldots, 1]^{\mathrm{T}}$. The conditions ensuring an order p are written in the form

$$\gamma(T_{ij})\mathbf{b}^{\mathrm{T}}\boldsymbol{\Phi}(T_{ij}) = 1, \quad i = 1,\ldots,p, \quad j = 1,\ldots,N_i, \tag{2.1}$$

where T_{ij} is a root tree of order i with an order number j and N_i is the number of trees of order i. The quantities $\gamma(T_{ij})$ and $\boldsymbol{\Phi}(T_{ij})$ were derived in [13]. Table 1 presents these quantities for trees up to the 4th order inclusively.

Definition 1. *The pseudo-stage order* of the Runge–Kutta method is the largest integer number $\overline{q}$ for which

$$\begin{gathered}\mathbf{b}^{\mathrm{T}}\mathbf{A}^k\left(\frac{\gamma(T_{i+1,j})}{i+1}\boldsymbol{\Phi}(T_{i+1,j}) - i\mathbf{Ac}^{i-1}\right) = 0, \quad 1 - i\mathbf{b}^{\mathrm{T}}\mathbf{c}^{i-1} = 0,\\ i = 1,\ldots,\overline{q}, \quad j = 1,\ldots,n_{i+1}, \quad k = 0,\ldots,s-1,\end{gathered} \tag{2.2}$$

where $T_{i+1,j}$ are trees of the $(i+1)$-st order with more than one branch issuing from the root vertex or the tree T_{21} if $i = 1$ (in Table 1, those are the trees T_{21}, T_{31}, T_{41}, and T_{42}) and n_{i+1} is the number of such trees of order $i+1$. Note that, if condition (2.2) is satisfied for $k = 0,\ldots,s-1$, then it is also satisfied for $k \geq s$ (this follows from the fact that the matrix $\mathbf{A}$ satisfies its characteristic equation).

Theorem 1. *The order p, the pseudo-stage order $\overline{q}$, and the stage order q of a Runge–Kutta method satisfy the inequality $p \geq \overline{q} \geq q$. Furthermore, if $1 - (\overline{q}+1)\mathbf{b}^{\mathrm{T}}\mathbf{c}^{\overline{q}} = 0$, then $p \geq \overline{q}+1$.*

Proof. With the ordering of trees adopted in [13], T_{i1} is a "bush" with $i-1$ branches issuing from the root, $\boldsymbol{\Phi}(T_{i1}) = \mathbf{c}^{i-1}$, and $\gamma(T_{i1}) = i$. It is clear from (2.2) that, for the trees T_{i1}, $i = 1,\ldots,\overline{q}$, conditions (2.1) are satisfied. For $i > 2$, $m = n_i + 1$, we have $\boldsymbol{\Phi}(T_{im}) = \mathbf{Ac}^{i-2}$ and $\gamma(T_{im}) = i(i-1)$. From (2.2), for $k = 0$, we obtain $\gamma(T_{i1})\mathbf{b}^{\mathrm{T}}\boldsymbol{\Phi}(T_{i1}) = \gamma(T_{im})\mathbf{b}^{\mathrm{T}}\boldsymbol{\Phi}(T_{im}) = 1$ and $\gamma(T_{ij})\mathbf{b}^{\mathrm{T}}\boldsymbol{\Phi}(T_{ij}) = \gamma(T_{im})\mathbf{b}^{\mathrm{T}}\boldsymbol{\Phi}(T_{im})$, $i = 3,\ldots,\overline{q}$, $j = 2,\ldots,n_i$, $m = n_i + 1$, which implies that the order conditions are satisfied for the trees T_{ij}, $i = 3,\ldots,\overline{q}$,

$j = 2,\ldots,n_i + 1$. For $\overline{q} \geq 3$, all conditions for the third order are satisfied. From the rule of calculating $\gamma(T)$, given in [13], it follows that, if T_i is a tree of order i and T_{i+1} is a tree for which $\boldsymbol{\Phi}(T_{i+1}) = \mathbf{A}\boldsymbol{\Phi}(T_i)$, then $\gamma(T_{i+1}) = (i+1)\gamma(T_i)$. Therefore, the conditions for the ith order and the conditions $1 - (i+1)\mathbf{b}^{\mathrm{T}}\mathbf{c}^i = 0$ and $\mathbf{b}^{\mathrm{T}}(\mathbf{c}^i - i\mathbf{A}\mathbf{c}^{i-1}) = 0$ (the latter is condition (2.2) for $j = 1$ and $k = 0$) imply that the order conditions are satisfied for all trees of the $(i+1)$-st order that have only one branch issuing from the root. For $i \geq 2$, these are the trees $T_{i+1,j}$, $j = n_{i+1} + 1,\ldots,N_{i+1} = n_{i+1} + n_i$. Since, for $\overline{q} \geq 3$, all the conditions for the third order are satisfied, we find, using mathematical induction, that the conditions for all orders $\overline{q}$ are also satisfied. In a similar manner, it can be proven that all conditions for the order $\overline{q} + 1$ are satisfied under the additional condition $1 - (\overline{q} + 1)\mathbf{b}^{\mathrm{T}}\mathbf{c}^{\overline{q}} = 0$.

Now let us prove that $\overline{q} \geq q$. For this, it suffices to show that, if $\overline{q} = q$, (1.5) implies (2.2). If conditions (1.5) are satisfied, then the conditions (2.2) for $i = 1,\ldots,q$, $j = 1$ will be satisfied too. From the inequality $p \geq q$ (which follows, e.g., from Theorem IV.5.1 [13]), it follows that all conditions (2.2) will also be satisfied for $i = 1,\ldots,q$, $j > 1$ (the proof is analogous to the proof given above). Examples of methods with $\overline{q} > q$ are given in [10, 11, 14] and in this paper.

Definition 2. The functions

$$e_{ij}(z) = z\mathbf{b}^{\mathrm{T}}(\mathbf{I} - z\mathbf{A})^{-1}\left(\frac{\gamma(T_{i+1,j})}{i+1}\boldsymbol{\Phi}(T_{i+1,j}) - i\mathbf{A}\mathbf{c}^{i-1}\right) + (1 - i\mathbf{b}^{\mathrm{T}}\mathbf{c}^{i-1}), \quad i \geq 1, \quad j = 1,\ldots,n_{i+1} \tag{2.3}$$

are called the error functions of the Runge–Kutta method.

In [12, 14], the error functions were obtained through local errors of the solution of simplest stiff equations as a function of $z = h\lambda$, where h is the step of the solution and λ is the coefficient on the right-hand side of the equation.

Theorem 2. *Conditions* (2.2) *and the condition*

$$e_{ij}(z) \equiv 0, \quad i = 1,\ldots,\overline{q}, \quad j = 1,\ldots,n_{i+1} \tag{2.4}$$

are equivalent.

Proof. $(\mathbf{I} - z\mathbf{A})^{-1}$ as a function of the matrix $z\mathbf{A}$ can be represented as a matrix polynomial of $z\mathbf{A}$ with a degree below s (see [15]). This implies that, if conditions (2.2) are satisfied, then conditions (2.4) are satisfied too. Now let us show that (2.4) implies (2.2). Let $e_{ij}(z) \equiv 0$. Write function (2.3) in the form $e_{ij}(z) = z\mathbf{b}^{\mathrm{T}}(\mathbf{I} - z\mathbf{A})^{-1}\mathbf{v} + (1 - i\mathbf{b}^{\mathrm{T}}\mathbf{c}^{i-1})$; then $1 - i\mathbf{b}^{\mathrm{T}}\mathbf{c}^{i-1} = 0$ and $\mathbf{b}^{\mathrm{T}}(\mathbf{I} - z\mathbf{A})^{-1}\mathbf{v} \equiv 0$. Using the equality $(\mathbf{I} - \mathbf{B})^{-1} = \mathbf{I} + \mathbf{B}(\mathbf{I} - \mathbf{B})^{-1}$, where $\mathbf{B} = z\mathbf{A}$ (it can be easily checked by multiplying both sided by $\mathbf{I} - \mathbf{B}$), we obtain $\mathbf{b}^{\mathrm{T}}(\mathbf{I} - z\mathbf{A})^{-1}\mathbf{v} = \mathbf{b}^{\mathrm{T}}\mathbf{v} + z\mathbf{b}^{\mathrm{T}}\mathbf{A}(\mathbf{I} - z\mathbf{A})^{-1}\mathbf{v}$, whence $\mathbf{b}^{\mathrm{T}}\mathbf{v} = 0$ and $\mathbf{b}^{\mathrm{T}}\mathbf{A}(\mathbf{I} - z\mathbf{A})^{-1}\mathbf{v} \equiv 0$. Continuing in a similar way and taking into account that all functions $\mathbf{b}^{\mathrm{T}}\mathbf{A}^k(\mathbf{I} - z\mathbf{A})^{-1}\mathbf{v}$ are bounded in the neighborhood of zero, we obtain $\mathbf{b}^{\mathrm{T}}\mathbf{A}^k\mathbf{v} = 0$, $k = 0,\ldots,s-1$, i.e., all conditions (2.2) are satisfied.

For solving stiff problems, it is advantageous to use strictly exact methods, in which $\mathbf{b}^{\mathrm{T}}$ is equal to the last row of the matrix $\mathbf{A}$. For such methods, formulas (2.2) and (2.3) can be simplified. Writing the condition of strict exactness in the form $\mathbf{b}^{\mathrm{T}} = \mathbf{e}_s^{\mathrm{T}}\mathbf{A}$, $\mathbf{e}_s^{\mathrm{T}} = [0,\ldots,0,1]$, and $c_s = 1$, we obtain from (2.2)

$$\mathbf{e}_s^{\mathrm{T}}\mathbf{A}^k\left(\frac{\gamma(T_{i+1,j})}{i+1}\boldsymbol{\Phi}(T_{i+1,j}) - i\mathbf{A}\mathbf{c}^{i-1}\right) = 0, \quad 1 - i\mathbf{b}^{\mathrm{T}}\mathbf{c}^{i-1} = 0,$$
$$i = 1,\ldots,\overline{q}, \quad j = 1,\ldots,n_{i+1}, \quad k = 1,\ldots,s.$$

Since the matrix $\mathbf{A}$ satisfies its characteristic equation, then the values of k can be shifted by setting $k = 0,\ldots,s-1$. In this case, for $j = 1$ and $k = 0$, we obtain $\mathbf{e}_s^{\mathrm{T}}(\mathbf{c}^i - i\mathbf{A}\mathbf{c}^{i-1}) = 1 - \mathbf{b}^{\mathrm{T}}\mathbf{c}^{i-1} = 0$; therefore, the condition $1 - i\mathbf{b}^{\mathrm{T}}\mathbf{c}^{i-1} = 0$ can be eliminated, as a result of which (2.2) will be replaced with

$$\mathbf{e}_s^{\mathrm{T}}\mathbf{A}^k\left(\frac{\gamma(T_{i+1,j})}{i+1}\boldsymbol{\Phi}(T_{i+1,j}) - i\mathbf{A}\mathbf{c}^{i-1}\right) = 0, \quad i = 1,\ldots,\overline{q}, \quad j = 1,\ldots,n_{i+1}, \quad k = 0,\ldots,s-1. \tag{2.5}$$

In order to obtain analogous formulas for $e_{ij}(z)$, successively substitute into (2.3) the relationships

$$z\mathbf{b}^{\mathrm{T}}(\mathbf{I}-z\mathbf{A})^{-1}=\mathbf{e}_s^{\mathrm{T}}(\mathbf{I}-z\mathbf{A})^{-1}-\mathbf{e}_s^{\mathrm{T}},\quad \gamma(T_{i+1,j})=(i+1)\prod_{l=1}^{k}\gamma(\tau_l)\quad \mathbf{e}_s^{\mathrm{T}}\boldsymbol{\Phi}(T_{i+1,j})=\mathbf{b}^{\mathrm{T}}\prod_{l=1}^{k}\boldsymbol{\Phi}(\tau_l),$$

where $\tau_1,\ldots,\tau_k$ are the trees obtained from the tree $T_{i+1,j}$ after removing the root with the edges incident to it (for example, for the tree T_{42} from Table 1, these are $\tau_1=T_1$ and $\tau_2=T_{21}$). Let $i\le p$; then, $\gamma(\tau_l)\mathbf{b}^{\mathrm{T}}\boldsymbol{\Phi}(\tau_l)=1$ and $i\mathbf{e}_s^{\mathrm{T}}\mathbf{A}\mathbf{c}^{i-1}=i\mathbf{b}^{\mathrm{T}}\mathbf{c}^{i-1}=1$. As a result of the corresponding substitutions, we obtain

$$e_{ij}(z)=\mathbf{e}_s{}^{\mathrm{T}}(\mathbf{I}-z\mathbf{A})^{-1}\left(\frac{\gamma(T_{i+1,j})}{i+1}\boldsymbol{\Phi}(T_{i+1,j})-i\mathbf{A}\mathbf{c}^{i-1}\right),\quad 1\le i\le p,\quad j=1,\ldots,n_{i+1}. \tag{2.6}$$

We will consider stiffly accurate methods with an explicit first stage, i.e., methods of the form (1.1) in which $\tilde{\mathbf{b}}^{\mathrm{T}}=\mathbf{e}_{s-1}^{\mathrm{T}}\tilde{\mathbf{A}}$. For such methods, for $\overline{q}>1$, condition (2.5) for the pseudo-stage order will be written in the form

$$\mathbf{e}_{s-1}^{\mathrm{T}}\tilde{\mathbf{A}}^k\left(\frac{\gamma(T_{i+1,j})}{i+1}\tilde{\boldsymbol{\Phi}}(T_{i+1,j})-i\tilde{\mathbf{A}}\tilde{\mathbf{c}}^{i-1}\right)=0,\quad i=2,\ldots,\overline{q},\quad j=1,\ldots,n_{i+1},\quad k=0,\ldots,s-2, \tag{2.7}$$

and error functions (2.6), in the form

$$e_{ij}(z)=\mathbf{e}_{s-1}^{\mathrm{T}}(\mathbf{I}-z\tilde{\mathbf{A}})^{-1}\left(\frac{\gamma(T_{i+1,j})}{i+1}\tilde{\boldsymbol{\Phi}}(T_{i+1,j})-i\tilde{\mathbf{A}}\tilde{\mathbf{c}}^{i-1}\right),\quad 2\le i\le p,\quad j=1,\ldots,n_{i+1}, \tag{2.8}$$

where the expression for $\tilde{\boldsymbol{\Phi}}(T_{i+1,j})$ is obtained by replacing $\mathbf{A}$ with $\tilde{\mathbf{A}}$ and $\mathbf{c}$ with $\tilde{\mathbf{c}}$. In comparison with (2.2) and (2.3), expressions (2.7) and (2.8) are simpler and more convenient for constructing methods with minimized or zero error functions.

3. FOUR-STAGE METHODS OF ORDERS 3 AND 4

Let us consider the construction of four-stage methods with an explicit first and one explicit internal stage having a stability function

$$R(z)=\frac{1+\beta_1 z+\beta_2 z^2}{1+\alpha_1 z+\alpha_2 z^2},\quad \alpha_1=-\frac{2}{3}+2\beta_2,\quad \alpha_2=\frac{1}{6}-\beta_2,\quad \beta_1=\frac{1}{3}+2\beta_2. \tag{3.1}$$

For $\beta_2=0$, this function specifies the Padé approximant of order 3 and, for $\beta_2=1/12$, the Padé approximation of order 4. The Butcher table of such methods has the form (1.1), where

$$\tilde{\mathbf{c}}=\begin{bmatrix}c_2\\ c_3\\ 1\end{bmatrix},\quad \tilde{\mathbf{A}}=\begin{bmatrix}a_{22} & a_{23} & a_{24}\\ a_{32} & a_{33} & a_{34}\\ a_{42} & a_{43} & a_{44}\end{bmatrix}.$$

Suppose that $q\ge 2$. Then,

$$a_{i1}=c_i-a_{i2}-a_{i3}-a_{i4},\quad a_{i2}=\frac{c_i^2-2(a_{i3}c_3+a_{i4}c_4)}{2c_2},\quad i=1,2,3. \tag{3.2}$$

To ensure the given stability function (3.1), the coefficients of the polynomial $\left|\mathbf{I}-z\tilde{\mathbf{A}}\right|=1+\alpha_1 z+\alpha_2 z^2+\alpha_3 z^3$ must satisfy the conditions

$$\alpha_1=-\frac{2}{3}+2\beta_2,\quad \alpha_2=\frac{1}{6}-\beta_2,\quad \alpha_3=-\left|\tilde{\mathbf{A}}\right|=0. \tag{3.3}$$

For $p=3$, conditions (3.3) uniquely define stability function (3.1), since the degree of its numerator is no higher than 3. Let us require that the methods constructed have $\overline{q}=3$. There are a total of two error functions of order 3: $e_{31}(z)=\mathbf{e}_{s-1}^{\mathrm{T}}(\mathbf{I}-z\tilde{\mathbf{A}})^{-1}(\tilde{\mathbf{c}}^3-3\tilde{\mathbf{A}}\tilde{\mathbf{c}}^2)$ and $e_{32}(z)=\mathbf{e}_{s-1}^{\mathrm{T}}(\mathbf{I}-z\tilde{\mathbf{A}})^{-1}(2\tilde{\mathbf{c}}(\tilde{\mathbf{A}}\tilde{\mathbf{c}})-3\tilde{\mathbf{A}}\tilde{\mathbf{c}}^2)$, but, for

$q = 2$, these functions are identical and, therefore, the corresponding conditions (2.7) are composed only from one of them and have the form

$$\mathbf{e}_{s-1}^{\mathrm{T}}\left(\tilde{\mathbf{c}}^3 - 3\tilde{\mathbf{A}}\tilde{\mathbf{c}}^2\right) = 0, \quad \tilde{\mathbf{b}}^{\mathbf{T}}\left(\tilde{\mathbf{c}}^3 - 3\tilde{\mathbf{A}}\tilde{\mathbf{c}}^2\right) = 0, \quad \tilde{\mathbf{b}}^{\mathbf{T}}\tilde{\mathbf{A}}\left(\tilde{\mathbf{c}}^3 - 3\tilde{\mathbf{A}}\tilde{\mathbf{c}}^2\right) = 0. \tag{3.4}$$

On the basis of conditions (3.2)–(3.4), a four-parameter family of methods with $q = 2$ and $\overline{q} = 3$ and stability function (3.1) were constructed. The specified parameters are β_2, c_2, c_3, and a_{33}. Expressions for the parameters of the method are rather cumbersome; therefore, here, only two subfamilies of this family, corresponding to $\beta_2 = 0$ and $\beta_2 = 1/12$, are presented.

Setting in (3.3) $\beta_2 = 0$, we obtain methods of order 3 with a stability function

$$R(z) = \frac{1 + z/3}{1 - (2/3)z + z/6}$$

(the same as the third-order Radau IIA method) and free coefficients c_2, c_3, and a_{33}. The remaining coefficients are found from formulas

$$c_4 = 1, \quad a_{34} = a_{33}c_3\frac{(2 - c_2 - c_3)(c_2 - c_3)}{(1 - c_2)^2} + \frac{c_3^2}{2}, \quad a_{44} = \frac{3c_2c_3 - 2(c_2 + c_3) + 1}{6(1 - c_2)(1 - c_3)},$$
$$a_{24} = c_2\frac{6(a_{33} + a_{44})(c_3 - c_2)(c_2 + c_3 - 2) + 3c_2c_3^2 - 6c_2c_3 + 4(c_2 - c_3) + 8c_3 - 5c_2}{6(1 - c_3)^2},$$
$$a_{23} = \frac{6c_2(a_{33} + a_{44}) - c_2(4 - 3c_2) - 6a_{24}}{6c_3}, \quad a_{43} = \frac{1 - c_2}{6c_3(c_3 - c_2)(1 - c_3)}, \tag{3.5}$$
$$a_{i2} = \frac{c_i^2 - 2(a_{i3}c_3 + a_{i4})}{2c_2}, \quad a_{i1} = c_i - a_{i2} - a_{i3} - a_{i4}, \quad i = 2,3,4,$$
$$a_{1j} = 0, \quad b_j = a_{4j}, \quad j = 1,\ldots,4.$$

Let us discuss the choice of the coefficient a_{33}. In the general case, the methods of family (3.5) have $q = 2$ and $\overline{q} = 3$. Specifying

$$a_{33} = c_3\frac{(2c_3 - 3)(c_2 - 1)}{6(c_3 - 1)(c_2 - c_3)}, \tag{3.6}$$

we obtain $q = \overline{q} = 3$. The presence of explicit stages can affect the stability of the internal stages. Consider the vector of stage stability functions $\mathbf{R}(z) = (\mathbf{I} - z\mathbf{A})^{-1}\mathbf{e}$. For large z, for the methods specified by formulas (3.5) and (3.6), the components of this vector are $R_i(z) \approx c_i(c_i - 1)^2 z$, which is quite understandable. All internal stability functions have a denominator as in (3.1), but, to ensure the third order of the internal stages, i.e., $q = 3$, degree of the the numerator must be no lower than 3. It is possible to avoid the instability of the internal stages for $q = 2$ and $\overline{q} = 3$. To do this, we should specify

$$a_{33} = \frac{(c_3 - 2)(c_2 - 1)}{6(c_3 - 1)(c_2 - c_3)}; \tag{3.7}$$

then, $R_i(\infty) = (c_i - 1)(3c_i - 1)$. The presence of unstable internal stages is not an obstacle to solving stiff problems if the final stage is stable. This is indicated by the results of testing of implicit and special explicit methods that have unstable internal stages and, at the same time, are very efficient in solving many stiff problems (see [9, 16]).

In the numerical experiments, we will estimate the effect of a higher stage order (with the same pseudo-stage order) and the instability of the internal stages. Therefore, we will take for the experiments two methods from family (3.5) in which we will set $c_2 = 1/3$ and $c_3 = 2/3$. The first of them (denote it by IERK33)

has $q = \overline{q} = 3$ and a_{33} from (3.6). The second method (IERK323) has $q = 2$, $\overline{q} = 3$, and a_{33} from (3.7). The coefficients of these methods are as follows:

IERK33

0	0	0	0	0
1/3	5/18	−7/36	7/18	−5/36
2/3	4/9	−5/9	10/9	−1/3
1	1/2	−3/4	3/2	−1/4

IERK323

0	0	0	0	0
1/3	5/18	−5/12	5/6	−13/36
2/3	4/9	−2/3	4/3	−4/9
1	1/2	−3/4	3/2	−1/4

For comparison, we will use the Radau IIA method of order 3 (denote it by Radau32).

Now let us consider methods of order 4, which we obtain by setting in (3.3) $\beta_2 = 1/12$. They have a stability function

$$R(z) = \frac{1 + z/2 + z^2/12}{1 - z/2 + z^2/12}$$

(the same as for the Gauss and Lobatto IIIA methods of order 4). Requiring that the method be symmetric (see [13] for symmetry conditions), we obtain a two-parameter family with free parameters α and β and the Butcher table

$$\begin{array}{c|cccc}
0 & 0 & 0 & 0 & 0 \\
\alpha & \beta - \dfrac{1 - 12\alpha^2 + 18\alpha^3 - 6\alpha^4}{12\alpha(1-\alpha)} & \dfrac{1}{12\alpha(1-\alpha)} - \beta & \dfrac{1}{12\alpha(1-\alpha)} - \beta & \beta - \dfrac{1 - 6\alpha^3 + 6\alpha^4}{12\alpha(1-\alpha)} \\
1-\alpha & \dfrac{1-\alpha^2}{2} - \beta & \beta & \beta & \dfrac{(1-\alpha)^2}{2} - \beta \\
1 & -\dfrac{1 - 6\alpha + 6\alpha^2}{12\alpha(1-\alpha)} & \dfrac{1}{12\alpha(1-\alpha)} & \dfrac{1}{12\alpha(1-\alpha)} & -\dfrac{1 - 6\alpha + 6\alpha^2}{12\alpha(1-\alpha)}
\end{array} \tag{3.8}$$

For $\alpha = (3 - \sqrt{3})/6$, we obtain Gaussian nodes, and table (3.8) defines a nested Gauss-type method, proposed in [7–9].

As in the third-order methods, the coefficient $\beta = a_{33}$ makes it possible to choose a method of a higher stage order or a method with stable internal stages. Setting

$$\beta = \frac{(1-\alpha)(1+2\alpha)}{12\alpha}, \tag{3.9}$$

we obtain a method of the third stage order with unstable internal stages, and setting

$$\beta = 1/(12\alpha), \tag{3.10}$$

a method of the second stage order with stable internal stages.

Since, in the fourth-order methods, $\overline{q} = 3 < p$, the effect of reduction in the order, although little, can be manifested. Therefore, it makes sense to analyze the fourth-order error functions. There are five of them:

$$e_{41}(z) = \mathbf{e}_s^{\mathrm{T}}(\mathbf{I} - z\mathbf{A})^{-1}\left(\mathbf{c}^4 - 4\mathbf{A}\mathbf{c}^3\right), \quad e_{42}(z) = \mathbf{e}_s^{\mathrm{T}}(\mathbf{I} - z\mathbf{A})^{-1}\left(2\mathbf{c}^2(\mathbf{A}\mathbf{c}) - 4\mathbf{A}\mathbf{c}^3\right),$$
$$e_{43}(z) = \mathbf{e}_s^{\mathrm{T}}(\mathbf{I} - z\mathbf{A})^{-1}\left(3\mathbf{c}\left(\mathbf{A}\mathbf{c}^2\right) - 4\mathbf{A}\mathbf{c}^3\right), \quad e_{44}(z) = \mathbf{e}_s^{\mathrm{T}}(\mathbf{I} - z\mathbf{A})^{-1}\left(6\mathbf{c}\left(\mathbf{A}^2\mathbf{c}\right) - 4\mathbf{A}\mathbf{c}^3\right),$$
$$e_{45}(z) = \mathbf{e}_s^{\mathrm{T}}(\mathbf{I} - z\mathbf{A})^{-1}\left(4(\mathbf{A}\mathbf{c})^2 - 4\mathbf{A}\mathbf{c}^3\right).$$

For any β, we have

$$e_{41}(z) = e_{42}(z) = e_{45}(z) = \frac{2\alpha(1-\alpha)z}{12 - 6z + z^2}. \tag{3.11}$$

The functions $e_{43}(z)$ and $e_{44}(z)$ have the same values for $q = 3$, i.e., for β in the form (3.9); for β in the form (3.10), we obtain

$$e_{43}(z) = e_{44}(z) = \frac{z}{2(12 - 6z + z^2)}. \tag{3.12}$$

Setting small α ensures small values of all the fourth-order error functions for $q = 3$ and functions (3.11) for $q = 2$. However, α should not be taken very small, because, in this case, the coefficients of the method become large, which can lead to an increase in the computational errors. We chose $\alpha = 1/30$; then the coefficient with largest absolute value is $a_{42} = a_{43} = -75/29$. The method obtained with $\alpha = 1/30$ and β specified by (3.9) is denoted by IERK43, and the method with $\alpha = 1/30$ and β specified by (3.10), by IERK423. Another pair of methods will be obtained on the basis of nested Gauss-type methods, i.e., by setting $\alpha = (3 - \sqrt{3})/6$. Specifying β by formula (3.9), we obtain the Kulikov43 method, and, using formula (3.10), the Kulikov423 method. With two different values of the parameters α and β, we can estimate the influence of these parameters on the efficiency of the method. For comparison, we use the Lobatto IIIA method of order 4, which will by denoted by Lobatto43. Note that this method can also be obtained from family (3.8) by setting $\alpha = 1/2$. Then, by any of formulas (3.9) or (3.10), we obtain $\beta = 1/6$. Substituting these α and β into (3.8), we obtain a method with identical second and third stages, and, excluding one of them, we obtain the Lobatto43 method.

4. METHODS OF ORDERS 5 AND 6

We will construct the methods of order 5 on the basis of the stability function in the form of the Padé approximation of order 5,

$$R(z) = \frac{60 + 24z + 3z^2}{60 - 36z + 9z^2 - z^3}.$$

Set $s = 5$, $q = 3$, and $\overline{q} = 4$. Then, along with conditions (1.5) for the stage order, we must satisfy the conditions

$$\left|\mathbf{I} - z\tilde{\mathbf{A}}\right| = 1 - \frac{3}{5}z + \frac{3}{20}z^2 - \frac{1}{60}z^3, \quad \mathbf{e}_{s-1}^{\mathrm{T}}\tilde{\mathbf{A}}^i(\tilde{\mathbf{c}}^4 - 4\tilde{\mathbf{A}}\tilde{\mathbf{c}}^3) = 0, \quad i = 0,\ldots,3.$$

We took $c_i = (i-1)/4$ and constructed two methods: IERK54 ($q = 4$, unstable internal stages) and IERK534 ($q = 3$, stable internal stages). The coefficients of these methods are as follows:

IERK54

0	0	0	0	0	0
1/4	413/2880	−1/1440	59/240	−271/1440	143/2880
1/2	53/360	7/90	7/15	−23/90	23/360
3/4	33/320	39/160	27/80	9/160	3/320
1	7/90	16/45	2/15	16/45	7/90

IERK534

0	0	0	0	0	0
1/4	31/225	−31/900	457/1200	−301/900	361/3600
1/2	271/1800	22/225	29/75	−38/225	61/1800
3/4	43/400	27/100	93/400	17/100	−3/100
1	7/90	16/45	2/15	16/45	7/90

For comparison, we use the Radau IIA method of order 5, which will be denoted by Radau53.

We also constructed a method of order 6 with the stability function

$$R(z) = \frac{1 + z/2 + z^2/10 + z^3/120}{1 - z/2 + z^2/10 - z^3/120}.$$

To obtain $\overline{q} = 5$, there must be at least two explicit internal stages, i.e., $s \geq 6$, but, in this case, we failed to construct a method with stable internal stages. We specified $s = 6$ and $q = \overline{q} = 5$ and determined the coefficients of the matrix $\mathbf{A}$ from conditions (1.5) and $\left|\mathbf{I} - z\tilde{\mathbf{A}}\right| = 1 - z/2 + z^2/10 - z^3/120$. From the sym-

metry condition, the vector of abscissas must have the form $\mathbf{c} = [0, \beta, \alpha, 1-\alpha, 1-\beta, 1]^{\mathrm{T}}$. To minimize the sixth-order error functions, we should set $\beta = -\alpha$. Then,

$$e_{6j}(z) = \frac{4\alpha^2(5\alpha^2 - 3)}{120 - 60z + 12z^2 - z^3}z,$$

and, for small α, these functions will also be small. We chose the value $\alpha = 0.1$, at which the coefficient table of the method has the form

0	0	0	0	0	0	0
−0.1	−131/1350	−1439/48000	24797/864000	−15133/864000	−449/48000	17/675
0.1	533/7425	−5261/528000	32533/864000	5803/864000	2029/528000	−149/14850
0.9	−369/275	72657/176000	45711/32000	44721/32000	75087/176000	−783/550
1.1	−1859/1350	20449/48000	1255133/864000	1215203/864000	21439/48000	−847/675
1	−73/54	5/12	155/108	155/108	5/12	−73/54

Demote the constructed method by IERK65. In the experiments, we also use the method of the sixth order from [7–9], which will be denoted by Kulikov634, and the Lobatto IIIA method (Lobatto64).

5. NUMERICAL EXPERIMENTS

In order to study the dependence of the error and the actual order on the stiffness of the problem, it is convenient to use tests with a known smooth solution independent on the stiffness parameter, which is proportional to the largest eigenvalue. Let us present the results of solving Kaps problem (1.2), which was used to study the convergence of methods as a function of the stiffness of the problem in [10–12, 17–19] and other works. The error e and estimated order $\tilde{p}$ are calculated by formulas (1.3) and (1.4). The calculations are performed with $h = 1/15$, $h_1 = 1/12$, and $h_2 = 1/18$ for the third- and fourth-order methods and, with $h = 1/10$, $h_1 = 1/8$, and $h_2 = 1/12$ for the methods orders 5 and 6. The results of the third-order methods are presented in Fig. 2; fourth-order methods, in Fig. 3; fifth-order methods, in Fig. 4; and sixth-order methods, in Fig. 1. Despite the different stage order, the third-order methods IERK33 and IERK323 demonstrate similar results, noticeably better than the results of Radau32. It was found that, among the fourth-order methods, the best one is the method with the minimized error functions, IERK43, and, among other methods, Kulikov43 and IERK423 are slightly better. Due to a higher pseudo-stage order, the errors of the fifth-order methods IERK54 and IERK534 are significantly smaller than those of Radau53. In this case, the behavior of the error of these methods near $\mu = 100$ is explained by the form of the error function

$$e_{51}(z) = -\frac{z(32 + 3z)}{32(60 - 36z + 9z^2 - z^3)},$$

which is equal to zero at $z = -32/3$. A small difference in the behavior of the errors is due to the fact that, in the IERK54 method, unlike IERK534, all error functions of the fifth order equal to each other. The most accurate among the sixth-order methods is IERK65, which has $\overline{q} = q = 5$, while, in the Kulikov634 and Lobatto64 methods, $\overline{q} = 4$.

The second stiff problem was taken from [20] and obtained by discretizing the diffusion equation $\partial u/\partial t = \partial^2 u/\partial x^2$, $0 \le x \le 1$, by the method of lines. The resulting system of ODEs has the form

$$y_i' = (N+1)^2(y_{i-1} - 2y_i + y_{i+1}), \quad i = 1, \ldots, N, \quad y_0 = 0, \quad y_{N+1} = \phi(t), \quad 0 \le t \le 1, \tag{5.1}$$

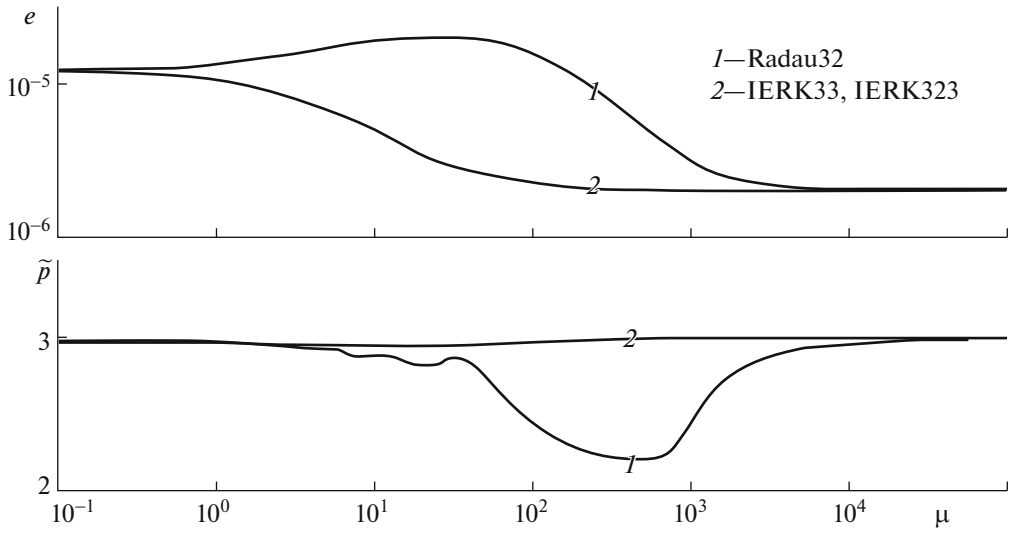

Fig. 2.

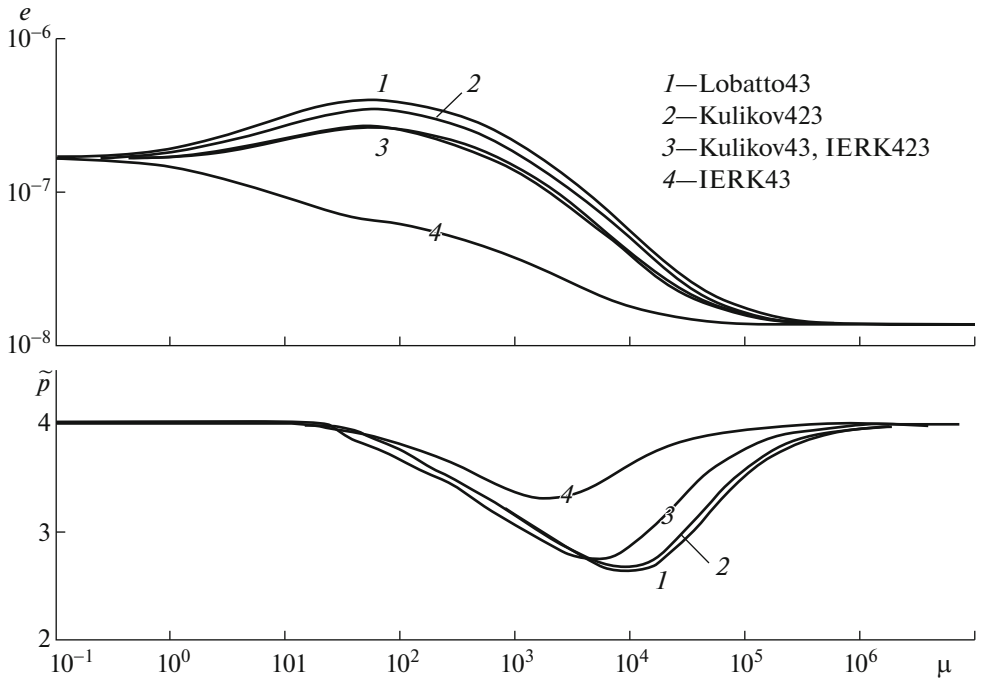

Fig. 3.

where

$$\phi(t) = ae^{-\nu t}\sin\left(\sqrt{2}\right) - e^{-\mu t}\sin(1), \quad a = \cos\left(\sqrt{2}\right)\Big/\left(\sqrt{2}\cos\left(2^{-1/2}\right)\right),$$
$$\mu = 2(N+1)^2\left(1-\cos\left(\frac{1}{N+1}\right)\right), \quad \nu = 2(N+1)^2\left(1-\cos\left(\frac{\sqrt{2}}{N+1}\right)\right),$$

and its exact solution is

$$y_i = ae^{-\nu t}\sin\left(\frac{\sqrt{2}i}{N+1}\right) - e^{-\mu t}\sin\left(\frac{i}{N+1}\right), \quad i = 1,\ldots,N.$$

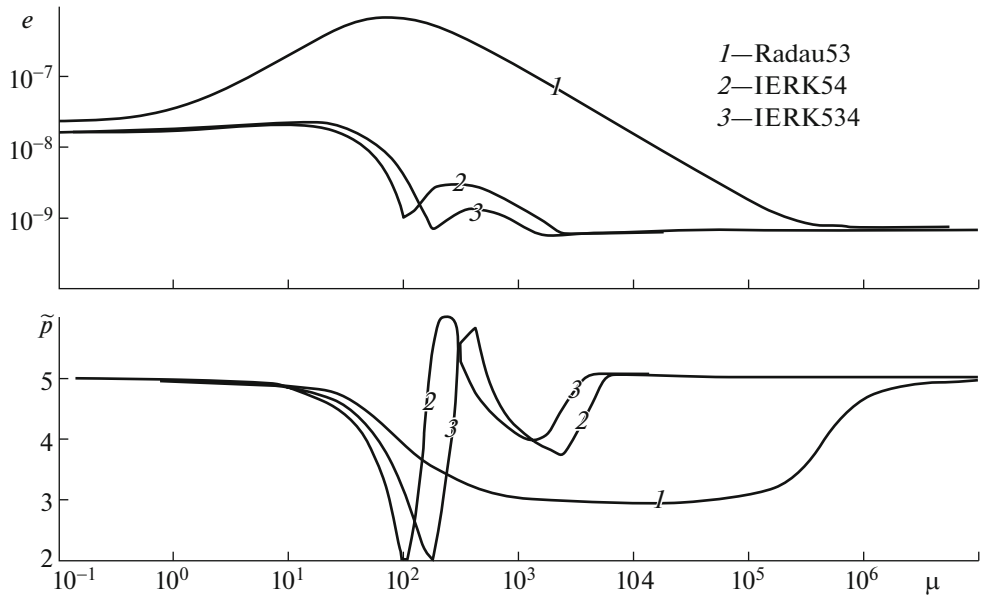

Fig. 4.

As in [20], we take $N = 10$. Then, the eigenvalues of the Jacobi matrix are located in the interval from –9.8 to –474.2.

The results of solving this problem (the maximum errors on the entire interval among all the components and the estimated order) are presented in Table 2. They agree with the results of solving the Kaps problem, except for the results of the IERK43 and IERK423 methods, which deserve a special comment. In solving problem (5.1), these methods demonstrated the same results, although, in solving the Kaps problem, IERK43 had a tangible advantage. This is explained by the fact that problem (5.1) is linear; therefore the expansion of its solution in the Taylor series does not contain elementary differentials that are present in nonlinear problems. The behavior of the error of solving linear nonautonomous problems can be analyzed on the basis of the error functions $e_{i1}(z)$ obtained by expanding the error of solving of the Prothero–Robinson equation in a Taylor series (see [12]). However, this is not enough to explain the behavior of the errors in nonlinear problems; it is also necessary to analyze the error functions $e_{ij}(z)$ for $j > 1$. In our case, it is sufficient to analyze formulas (3.11) and (3.12). The IERK43 and IERK423 methods have the same error function $e_{41}(z)$, which is expressed by formula (3.11). Therefore, when solving linear problem (5.1), they demonstrate practically the same results. However, for the IERK423 method, we have $e_{43}(z)/e_{41}(z) \equiv 225/29$, whereas, for the IERK43, $e_{43}(z) \equiv e_{41}(z)$, which explains the tangible advantage of the IERK43 method in solving the Kaps problem. A similar explanation can be given to the same results demonstrates by the Kulikov43 and Kulikov423 methods in solving problem (5.1) and a slight advantage of the first of them over the second in solving the Kaps problem.

Thus, the results of solving stiff problems presented above are fully explained with the help of pseudo-stage order and error functions. The pseudo-stage order has a decisive influence on the accuracy of solution. Among methods with equal q, the more accurate one is that having a greater $\overline{q}$, and, among methods with equal $\overline{q}$, the more accurate one is that has smaller values of the error function of order $\overline{q}+1$.

Now let us analyze the convergence of methods for solving differential-algebraic equations of higher indices. The problem of index 2

$$y_1' = -(y_1 y_2 z)^{1/4}, \quad y_2' = -y_1\left(y_1^2 + y_2\right)/z, \quad 0 = y_1^2 - y_2,$$
$$y_1(0) = y_2(0) = z(0) = 1, \quad 0 \le t \le 1 \tag{5.2}$$

Table 2

Method	Error		$\tilde{p}$
	$h_1 = 0.25$	$h_2 = 0.025$	
Radau32	2.90×10^{-5}	4.72×10^{-8}	2.79
IERK33	1.01×10^{-5}	1.57×10^{-8}	2.81
IERK323	1.01×10^{-5}	1.57×10^{-8}	2.81
Lobatto43	5.60×10^{-6}	7.24×10^{-10}	3.89
Kulikov43	4.06×10^{-6}	4.95×10^{-10}	3.91
Kulikov423	4.06×10^{-6}	4.95×10^{-10}	3.91
IERK43	1.67×10^{-6}	1.56×10^{-10}	4.03
IERK423	1.67×10^{-6}	1.56×10^{-10}	4.03
Radau53	1.57×10^{-6}	1.56×10^{-10}	4.00
IERK54	1.73×10^{-7}	2.95×10^{-12}	4.77
IERK534	1.73×10^{-7}	2.95×10^{-12}	4.77
Lobatto64	1.10×10^{-7}	9.10×10^{-13}	5.08
Kulikov634	9.35×10^{-8}	7.62×10^{-13}	5.09
IERK65	3.31×10^{-9}	3.16×10^{-15}	6.02

Table 3

Method	e_y	e_z	$\tilde{p}_y$	$\tilde{p}_z$
Radau32	2.04×10^{-6}	6.54×10^{-4}	3.00	1.99
IERK33	2.75×10^{-6}	7.13×10^{-6}	3.00	2.98
IERK323	2.06×10^{-6}	3.06×10^{-6}	3.01	3.02
Lobatto43	2.10×10^{-8}	3.01×10^{-4}	4.00	2.00
Kulikov43	6.68×10^{-6}	2.12×10^{-4}	2.00	2.00
Kulikov423	3.33×10^{-8}	2.58×10^{-4}	4.00	2.00
IERK43	3.50×10^{-5}	2.26×10^{-5}	2.00	2.00
IERK423	4.87×10^{-8}	1.89×10^{-4}	4.00	2.00
Radau53	1.52×10^{-10}	8.64×10^{-6}	5.00	2.99
IERK54	3.91×10^{-7}	2.28×10^{-7}	2.97	3.15
IERK534	2.14×10^{-10}	3.87×10^{-8}	5.00	3.99
Lobatto64	1.04×10^{-12}	1.58×10^{-7}	5.99	3.98

has the solution $y_1(t) = z(t) = e^{-t}$, $y_2(t) = e^{-2t}$, and the problem of index 3

$$\begin{gathered} y_1' = -(y_1y_2z_1z_2)^{1/6}, \quad y_2' = y_1(y_2 - 3z_2)/z_1, \\ z_1' = -z_1z_2u/(y_1y_2), \quad z_2' = -(y_1y_2 + z_1z_2)/u, \\ 0 = y_1^2 - y_2, \quad y_1(0) = y_2(0) = z_1(0) = z_2(0) = u(0) = 1, \quad 0 \le t \le 1 \end{gathered} \tag{5.3}$$

has the solution $y_1(t) = z_1(t) = u(t) = e^{-t}$, $y_2(t) = z_2(t) = e^{-2t}$. The errors and estimated orders are calculated by formulas (1.3) and (1.4) with $h = h_1 = 1/20$ and $h_2 = 1/40$ for each of the following components of

Table 4

Method	e_y	e_z	e_u	$\tilde{p}_y$	$\tilde{p}_z$	$\tilde{p}_u$
Radau32	9.94×10^{-6}	4.63×10^{-4}	2.43×10^{-2}	1.96	1.97	0.95
IERK33	1.30×10^{-7}	5.07×10^{-6}	6.02×10^{-4}	3.04	3.00	1.96
IERK323	7.86×10^{-7}	1.83×10^{-6}	4.61×10^{-4}	3.01	2.93	1.96
Radau53	2.01×10^{-9}	6.10×10^{-6}	5.03×10^{-4}	4.08	2.97	1.99
IERK54	8.04×10^{-8}	7.40×10^{-7}	7.94×10^{-6}	2.99	2.98	2.99
IERK534	1.60×10^{-10}	2.71×10^{-8}	6.56×10^{-6}	5.00	3.96	2.99
Lobatto64	1.21×10^{-9}	8.77×10^{-8}	4.63×10^{-4}	3.98	3.97	2.00

the solution: $\mathbf{y} = (y_1, y_2)$, the y-component (variables of index 1); $\mathbf{z} = (z_1, z_2)$, the z-component (variables of index 2); and u, the u-component (a variable of index 3). The results of the solution of problem (5.2) are presented in Table 3, and of problems (5.3), in Table 4. If the method does not converge (one of the estimates of the order is about zero or negative), then its results are not given. Similar results were also obtained in solving problems of indices 2 and 3 in [21, 22].

Among the third-order methods, the most advantageous are the methods of a higher pseudo-stage order, IERK33 and IERK323. All fourth-order methods proved to be unsuitable for solving problems of index 3. This is probably due to the fact that they have $R(\infty) = 1$, which leads to accumulation of errors. Among the fifth-order methods, the best results were demonstrated by IERK534, a method with a stable internal stage. Of all the sixth-order methods, only Lobatto64 provided convergence, but it has $R(\infty) = -1$, which can lead to deterioration of convergence in the integration with a variable step (see Remark 2 to Theorem 5.2 in [21]).

6. CONCLUSIONS

The results of the experiments have shown that the methods with explicit internal stages can be more accurate than the analogous methods (of the same order and with the same stability function) without explicit internal stages. Such methods can have an advantage in solving large problems with sufficiently simple right-hand sides, when the main computational costs are caused by solving a system of linear algebraic equations in each iteration.

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