# Investigation of (m,2)-methods for Solving Stiff Problems 

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#### Abstract

A family of (m,2)-methods for stiff problems solving is studied. Numerical schemes of the second and the third order are constructed. It is shown, that a maximum order of ( $\mathrm{m}, 2$ )-methods is four. A-stable and L-stable numerical formulas of a maximum order are designed. An inequality for accuracy control for the L-stable methods of the fourth order is constructed. Numerical results confirming the efficiency of the constructed method are given.


Keywords- stiff system, a class of (m,k)-methods, L-stability, accuracy control of calculations.

## I. Introduction

When solving the Cauchy problem for a stiff system of ordinary differential equations, Rosenbrock type methods [1] are widely used due to simple implementation and reasonably good accuracy and stability. The Rosenbrock type methods where the same Jacobi matrix is used in calculating each stage are in the most common use. It is known (see, e.g., [2]), that in this case the maximum accuracy order of the $m$-stage Rosenbrock method is $(m+1)$, in addition, a scheme of the maximum order can be only $A$ stable. If the maximum order is not required, a $L$-stable numerical formula of order $m$ can be constructed. In practical calculations, as a rule, the maximum order is abandoned in favour of $L$-stability.

A scheme of order higher than two with the Jacobi matrix freezing can not be constructed on the basis of methods of the Rosenbrock type [3]. This limits the application of these methods to calculations with moderate accuracy or to problems of a small dimension.

In [4-5] a class of $(m, k)$-methods where determining a stage does not involve calculation of a right-hand part of a system of differential equations is proposed. The implementation of $(m, k)$-methods is as simple as that of Rosenbrock methods, however, ( $m, k$ )-schemes have advantages for accuracy and stability. In the framework of ( $m, k$ ) -methods the problem of freezing the Jacobi matrix and its numerical approximation is solved more easily.

[^0]In this paper $(m, 2)$-methods for solving stiff systems where at each step the right-hand part of a system of ordinary differential equations is calculated two times are investigated. It is shown that the maximum order of accuracy of the $L$ stable $(m, 2)$-method is four. An inequality for accuracy control for the $L$-stable methods of the fourth order is constructed. Numerical results confirming the efficiency of the constructed method are given.

## II. METHODS OF Rosenbrock Type

We consider a Cauchy problem for a system of ordinary differential equations
$y^{\prime}=f(t, y), y\left(t_{0}\right)=y_{0}, t_{0} \leq t \leq t_{k}$,
where $y$ and $f$ are real $N$-dimensional vector functions, $t$ is an independent variable, which varies over the given finite interval. It is known, that introducing an additional variable one can reduce a non-autonomous system to an autonomous form. Hence, the formulation of (1) can be considered without the loss of generality. Methods of a Rosenbrock type for problem (1) have the form
$y_{n+1}=y_{n}+\sum_{i=1}^{m} p_{i} k_{i}$,
$D_{n} k_{i}=h f\left(y_{n}+\sum_{j=1}^{i-1} \beta_{i j} k_{j}\right)$,
$D_{n}=E-a h f_{n}^{\prime}$,
where $h$ is an integration step, $E$ is an identity matrix, $f_{n}^{\prime}=\partial f\left(y_{n}\right) / \partial y$ is the Jacobi matrix of a vector function $f(y), a, p_{i}, 1 \leq i \leq m$, and $\beta_{i j}, 1 \leq i \leq m, 1 \leq j \leq i-1$, are numerical coefficients. At present, the methods of a Rosenbrock type are treated in a wider sense [2]. Numerical formula (2) can be obtained from a class of semi-explicit methods of a Runge-Kutta type provided that only one iteration step of the Newton's method is performed when calculating each stage. In Rosenbrock methods only linear systems of algebraic equations are solved when calculating a stage, whereas in implicit or semi-explicit Runge-Kutta methods an iterative process of the Newton type is required that leads to additional problems in its implementation.

## III. The CLASS OF (M, K)-METHODS

A class of $(m, k)$-methods [4] is introduced as follows. Let integer positive numbers $m$ and $k, k \leq m$, be given. Denote a set of integer numbers $i, 1 \leq i \leq m$, by $M_{m}$ and the subsets of $M_{m}$ of the form
$M_{k}=\left\{m_{i} \in M_{m} \mid 1=m_{1}<\cdots<m_{k} \leq m\right\}$,
$J_{i}=\left\{m_{j-1} \in M_{m} \mid j>1, m_{j} \in M_{k}, m_{j} \leq i\right\}$,
$2 \leq i \leq m$,
by $M_{k}$ and $J_{i}$. Then, $(m, k)$-methods can be represented in the form
$y_{n+1}=y_{n}+\sum_{i=1}^{m} p_{i} k_{i}, D_{n}=E-a h f_{n}^{\prime}$,
$D_{n} k_{i}=h f\left(y_{n}+\sum_{j=1}^{i-1} \beta_{i j} k_{j}\right)+\sum_{j \in J_{i}} \alpha_{i j} k_{j}, i \in M_{k}$,
$D_{n} k_{i}=k_{i-1}+\sum_{j \in J_{i}} \alpha_{i j} k_{j}, \quad i \in M_{m} \backslash M_{k}$.
The set $J_{i}, 2 \leq i \leq m$, serves to eliminate the redundant coefficients $\alpha_{i j}$ by means of which we can not make effect on accuracy and stability of (4) and which can be expressed linearly in terms of other coefficients. In traditional one-step methods, to determine computational work per integration step a single constant $m$ being the number of stages is sufficient because in these methods each stage is accompanied by obligatory calculation of the right-hand part of (1). In methods (4) there are two types of stages. For some stages it is necessary to calculate the right-hand part, but for other ones it is not required. As a result, to determine computational work per step in (4) two constants $m$ and $k$ are needed. The expense of a step is as follows: the Jacobi matrix is calculated once and the decomposition of a matrix $D_{n}$ is performed once, function $f$ is calculated $k$ times, backward Gauss is performed $m$ times. For $k=m$ and $\alpha_{i j}=0$ numerical schemes (4) coincide with methods (2) of a Rosenbrock type. In other cases these methods differ and methods (4) have advantages over methods (2).

## IV. The Maximal Order of Accuracy of (M,2)-methods

We consider $(m, 2)$-methods of the following form
$y_{n+1}=y_{n}+\sum_{i=1}^{m} p_{i} k_{i}$,
$D_{n}=E-a h f_{n}^{\prime}$,
$D_{n} k_{1}=h f\left(y_{n}\right), D_{n} k_{i}=k_{i-1}, 2 \leq i \leq s_{1}-1$,
$D_{n} k_{s_{1}}=h f\left(y_{n}+\sum_{j=1}^{s_{1}-1} \beta_{s_{1}, j} k_{j}\right)+\alpha_{s_{1}, s_{1}-1} k_{s_{1}-1}$,
$D_{n} k_{i}=k_{i-1}+\alpha_{i, s_{1}-1} k_{s_{1}-1}, s_{1}+1 \leq i \leq m$,
where $s_{1}$ and $m, s_{1} \leq m$, are arbitrary integer constants. It is easy to see, that formulas (5) describe all kinds of $(m, 2)$ methods (4).

Theorem. For any number $m$ of stages and for any set $M_{2}$ it is impossible to construct an $(m, 2)$-method of accuracy of order higher than four.
Without the loss of generality we give a proof for scalar problem (1), which exact solution $y\left(t_{n+1}\right)$ can be written in the form

$$
\begin{align*}
y\left(t_{n+1}\right) & =y\left(t_{n}\right)+h f+\frac{1}{2} h^{2} f^{\prime} f \\
& +\frac{1}{6} h^{3}\left[f^{\prime 2} f+f^{\prime \prime} f^{2}\right] \\
& +\frac{1}{24} h^{4}\left[f^{\prime 3} f+4 f^{\prime} f^{\prime \prime} f^{2}+f^{\prime \prime \prime \prime} f^{3}\right]  \tag{6}\\
& +\frac{1}{120} h^{5}\left[f^{\prime 4} f+4 f^{\prime} f^{\prime \prime \prime} f^{3}+5 f^{\prime 2} f^{\prime \prime \prime} f^{2}+f^{\prime \prime 2} f^{3}+f^{I V} f^{4}\right] \\
& +O\left(h^{6}\right)
\end{align*}
$$

where the elementary differentials are calculated on an exact solution $y\left(t_{n}\right)$. We consider $(m, 2)$-methods (5). Taking into account

$$
\begin{align*}
D_{n}^{-1} & =E+a h f_{n}^{\prime}+a^{2} h^{2} f_{n}^{\prime 2}+a^{3} h^{3} f_{n}^{\prime 3} \\
& +a^{4} h^{4} f_{n}^{\prime 4}+O\left(h^{5}\right), \tag{7}
\end{align*}
$$

we observe that the second calculation of a function $f(y)$ is performed at the point

$$
y_{n, c}=y_{n}+\sum_{j=1}^{s_{1}-1} \beta_{s_{1}, j} k_{j}=y_{n}+\sum_{i=1}^{5} c_{i} h^{i} f_{n}^{\prime(i-1)} f_{n}+O\left(h^{6}\right)
$$

where $c_{i}, 1 \leq i \leq 4$, are determined in terms of the coefficients of scheme (5) and the elementary differentials are calculated on an approximate solution $y_{n}$. Taking into consideration (6) and (7), to prove the theorem it is sufficient to show that the Taylor expansion of the function $f\left(y_{n, c}\right)$ in terms of powers of $h$ does not involve the term $h^{5} f_{n}^{\prime \prime 2} f_{n}^{3}$. The Taylor expansion of $f\left(y_{n, c}\right)$ in a vicinity of the point $y_{n}$ up to terms of order $h^{5}$ inclusive has the form

$$
\begin{aligned}
& f\left(y_{n, c}\right)=h f_{n}+c_{1} h^{2} f_{n}^{\prime} f_{n}+h^{3}\left[c_{2} f_{n}^{\prime 2} f_{n}+\frac{1}{2} f_{n}^{\prime \prime} f_{n}^{2}\right] \\
& \quad+h^{4}\left[c_{3} f_{n}^{\prime 3} f_{n}+c_{1} c_{2} f_{n}^{\prime} f_{n}^{\prime \prime} f_{n}^{2}+\frac{1}{6} c_{1}^{3} f_{n}^{\prime \prime \prime} f_{n}^{3}\right] \\
& \quad+h^{5}\left[c_{4} f_{n}^{\prime 4} f_{n}+c_{1} c_{3} f_{n}^{\prime 3} f_{n}^{\prime \prime} f_{n}^{2}+\frac{1}{2} c_{1}^{2} c_{2} f_{n}^{\prime} f_{n}^{\prime \prime \prime} f_{n}^{3}+\frac{1}{24} c_{1}^{4} f_{n}^{I V} f_{n}^{4}\right] \\
& \quad+O\left(h^{6}\right)
\end{aligned}
$$

which completes the proof.

## V. An A-stable (M,2)-Method of Order Four

Let $k=2$. Take $M_{k}=\{1,2\}$, then $J_{i}=\{1\}, 2 \leq i \leq m$. As a result, we obtain the numerical schemes of the form
$y_{n+1}=y_{n}+\sum_{i=1}^{m} p_{i} k_{i}$,
$D_{n} k_{1}=h f\left(y_{n}\right)$,
$D_{n} k_{2}=h f\left(y_{n}+\beta_{21} k_{1}\right)+\alpha_{21} k_{1}$,
$D_{n} k_{i}=k_{i-1}+\alpha_{i 1} k_{1}, 3 \leq i \leq m$.
Case 1. Let $m=2$. Then the coefficients
$a=\frac{6+\sqrt{12}}{12}, p_{1}=\frac{76 a-3}{54 a}, p_{2}=\frac{16}{27}$,
$\beta_{21}=\frac{3}{4}, \alpha_{21}=\frac{3-54 a}{32 a}$
provide the third order of the $A$-stable scheme (8). Usually the maximal order is abandoned in favour of $L$-stability. For $m=2$ the coefficients of the second order $L$-stable scheme have the form
$a=\beta_{21}=1-\frac{\sqrt{2}}{2}, p_{1}=a, p_{2}=1-a, \alpha_{21}=0$.
Case 2. Let $m=3$. Introduce the notations
$c_{1}=1-4 a+2 a^{2}, c_{2}=\beta_{21}+a \alpha_{21}$,
$c_{3}=6 a c_{2} \beta_{21}^{2}, c_{4}=2 c_{2}\left(\beta_{21}-a\right)$,
$c_{5}=3 c_{1} \beta_{21}^{2}\left(\beta_{21}-a\right)$.
Then the coefficients
$p_{1}=\frac{a c_{3}+c_{4}-c_{5}}{c_{3}}$,
$p_{2}=\frac{2 c_{2}-3 \beta_{21}^{2} c_{1}}{6 \beta_{21}^{2} c_{2}}, p_{3}=\frac{c_{1}}{2 c_{2}}$,
$\alpha_{31}=\frac{2 c_{2}\left[(1-a) c_{3}-c_{4}+c_{5}-2 a c_{2}\left(1+\alpha_{21}\right)\right]}{c_{2} c_{3}}$.
provide third accuracy order of the $L$-stable scheme (8). Here, $\alpha_{21}$ and $\beta_{21}$ are constant coefficients and the value of $a$ is determined from the equation $6 a^{3}-18 a^{2}+9 a-1=0$.

It is easy to verify that for any value of $m$ it is impossible to construct an $L$-stable scheme (8) of the fourth order. To do this, it is sufficient to write conditions of the fourth accuracy order consistency and $L$-stability. The simplest study of the obtained nonlinear system of algebraic equations shows its incompatibility. However, provided $L$-stability is not required, the method (8) of fourth accuracy order can be constructed.

Case 3. Let $m=4$. Introduce the notations

$$
\begin{aligned}
& c_{1}=\frac{60-81 c_{7}}{81}, c_{2}=\frac{18-324 c_{7}}{81} \\
& c_{3}=\frac{405 c_{7}-64}{81}, c_{4}=\frac{19-162 c_{7}}{81}
\end{aligned}
$$

$c_{5}=\frac{64-81 c_{7}}{81}, c_{6}=\frac{162 c_{7}-16}{81}$,
where $c_{7} \neq 0$ is a constant coefficient. Then the coefficients of the fourth order method have the form
$a=\frac{3}{8}, \beta_{21}=\frac{3}{4}, p_{1}=c_{1}, p_{2}=c_{5}, p_{3}=c_{6}$,
$p_{4}=c_{7}, \alpha_{21}=\frac{c_{4}}{c_{7}}, \alpha_{31}=\frac{c_{3} c_{7}-c_{4} c_{6}}{c_{7}^{2}}$,
$\alpha_{41}=\frac{c_{2} c_{7}^{2}-c_{4} c_{5} c_{7}-c_{3} c_{6} c_{7}+c_{4} c_{6}^{2}}{c_{7}^{2}}$.

## VI. An L-Stable (M,2)-METHOD of Order Four

Let $k=2$. Take $M_{k}=\{1,3\}$, then $J_{i}=\{2\}, 3 \leq i \leq 4$. As a result, we get a scheme of the form
$y_{n+1}=y_{n}+\sum_{i=1}^{4} p_{i} k_{i}$,
$D_{n} k_{1}=h f\left(y_{n}\right), D_{n} k_{2}=k_{1}$,
$D_{n} k_{3}=h f\left(y_{n}+\beta_{31} k_{1}+\beta_{32} k_{2}\right)+\alpha_{32} k_{2}$,
$D_{n} k_{4}=k_{3}+\alpha_{42} k_{2}$.
Construct an $L$-stable method of order four. To do this, substitute the expansion of the stages $k_{i}, 1 \leq i \leq 4$, in the Taylor series in the first formulae of (9). Assuming that $y_{n}=y\left(t_{n}\right)$ and comparing the obtained presentation of the approximate solution $y_{n+1}$ with the Taylor expansion of the exact solution $y\left(t_{n+1}\right)$, write the conditions of the fourth accuracy order

$$
\begin{aligned}
& p_{1}+p_{2}+\left(1+\alpha_{32}\right) p_{3}+\left(1+\alpha_{32}+\alpha_{42}\right) p_{4}=1, \\
& a p_{1}+2 a p_{2}+\left(a+\beta_{31}+\beta_{32}+3 a \alpha_{32}\right) p_{3} \\
& \quad+\left(2 a+\beta_{31}+\beta_{32}+4 a \alpha_{32}+3 a \alpha_{42}\right) p_{4}=\frac{1}{2}, \\
& a^{2} p_{1}+3 a^{2} p_{2}+\left(a^{2}+2 a \beta_{31}+3 a \beta_{32}+6 a^{2} \alpha_{32}\right) p_{3}+ \\
& \quad+\left(3 a^{2}+3 a \beta_{31}+4 a \beta_{32}+10 a^{2} \alpha_{32}+6 a^{2} \alpha_{42}\right) p_{4}=\frac{1}{6}, \\
& \quad a^{3} p_{1}+4 a^{3} p_{2}+\left(a^{3}+3 a^{2} \beta_{31}+6 a^{2} \beta_{32}+10 a^{3} \alpha_{32}\right) p_{3} \\
& \quad+\left(4 a^{3}+6 a^{2} \beta_{31}+10 a^{2} \beta_{32}+20 a^{3} \alpha_{32}+10 a^{3} \alpha_{42}\right) p_{4}=\frac{1}{24}, \\
& \left(\beta_{31}+\beta_{32}\right)^{2}\left(p_{3}+p_{4}\right)=\frac{1}{3}, \\
& a\left(\beta_{31}+\beta_{32}\right)\left(\beta_{31}+2 \beta_{32}\right)\left(p_{3}+p_{4}\right)=\frac{1}{8}, \\
& a\left(\beta_{31}+\beta_{32}\right)^{2}\left(\frac{1}{2} p_{3}+p_{4}\right)=\frac{1}{24}, \\
& \left(\beta_{31}+\beta_{32}\right)^{3}\left(p_{3}+p_{4}\right)=\frac{1}{4} .
\end{aligned}
$$

Applying the method (9) to the solution of the test problem $y^{\prime}=\lambda y, y(0)=y_{0}, t \geq 0$,
obtain the condition of $L$-stability of the numerical formulae (9) of the form
$a\left(a-p_{1}\right)+\left(\beta_{31}-a\right) p_{3}=0$.
Investigating the consistency of this relation and the order conditions, write
$p_{1}=\frac{76 a^{2}-29 a+3}{27 a^{2}}, p_{2}=\frac{146 a^{2}+89 a-12}{27 a^{2}}$,
$p_{3}=\frac{32 a-4}{27 a}, p_{4}=\frac{4-16 a}{27 a}, \beta_{31}=\frac{48 a-9}{32 a}$,
$\beta_{32}=\frac{9-24 a}{32 a}, \alpha_{32}=\frac{-54 a^{2}+57 a-12}{8 a-32 a^{2}}$,
$\alpha_{42}=\frac{-864 a^{3}+828 a^{2}-288 a+36}{a(4-16 a)^{2}}$,
where $a$ is determined from the necessary condition of $L$-stability
$24 a^{4}-96 a^{3}+72 a^{2}-16 a+1=0$.
The given equation have four real roots
$a_{1}=0.10643879214266, a_{2}=0.22042841025921$,
$a_{3}=0.57281606248213, a_{4}=3.10031673511599$.
In calculations it is wise to take $a=0.57281606248213$, and the coefficients of the scheme (9) have the form
$p_{1}=1.27836939012447, p_{2}=-1.00738680980438$,
$p_{3}=0.92655391093950, p_{4}=-0.33396131834691$,
$\beta_{31}=1.00900469029922, \beta_{32}=-0.25900469029921$,
$\alpha_{32}=-0.49552206416578, \alpha_{42}=-1.28777648233922$.

## VII. ACCURACY CONTROL

The third accuracy order method of the form
$y_{n+1,1}=y_{n}+b_{1} k_{1}+b_{2} k_{2}+b_{3} k_{3}+b_{4} k_{5}$
can be applied for accuracy control of numerical formula (9) of the fourth order. Here, $D_{n} k_{5}=k_{4}$, and $k_{i}, 1 \leq i \leq 3$, are determined in (9). It is easy to see, that the third order requirements have the form

$$
\begin{aligned}
& b_{1}+b_{2}+\left(1+\alpha_{32}\right) b_{3}+\left(1+\alpha_{32}+\alpha_{42}\right) b_{4}=1 \\
& a b_{1}+2 a b_{2}+\left(a+\beta_{31}+\beta_{32}+3 a \alpha_{32}\right) b_{3} \\
& \quad+\left(3 a+\beta_{31}+\beta_{32}+5 a \alpha_{32}+4 a \alpha_{42}\right) b_{4}=\frac{1}{2}, \\
& a^{2} b_{1}+3 a^{2} b_{2}+\left(a^{2}+2 a \beta_{31}+3 a \beta_{32}+6 a^{2} \alpha_{32}\right) b_{3} \\
& \quad+\left(6 a^{2}+4 a \beta_{31}+5 a \beta_{32}+15 a^{2} \alpha_{32}+10 a^{2} \alpha_{42}\right) b_{4}=\frac{1}{6}, \\
& \left(\beta_{31}+\beta_{32}\right)^{2}\left(b_{3}+b_{4}\right)=\frac{1}{3},
\end{aligned}
$$

where the coefficients $a, \beta_{31}, \beta_{32}, \alpha_{32}$ and $\alpha_{42}$ are set in (10). The given system is linear with respect to $b_{i}, 1 \leq i \leq 4$. As a result, we have
$b_{1}=1.203100567018353$,
$b_{2}=-6.552116304144386 \cdot 10^{-1}$,
$b_{3}=7.115271884598151 \cdot 10^{-1}$,
$b_{4}=-1.189345958672225 \cdot 10^{-1}$.
Now, we can calculate an error estimation $\varepsilon_{n}$ by the formula $\varepsilon_{n}=\left\|y_{n+1}-y_{n+1,1}\right\|$,
and verify the inequality $\varepsilon_{n} \leq \varepsilon$ on a choice of an integration step size, where $\|\cdot\|$ is some norm in $R^{N}, \varepsilon$ is accuracy of calculations.

## VIII. THE RESULTS OF CALCULATIONS

The following example describes a system of two differential equations in partial derivatives with initial and boundary conditions. The Akzo Nobel Central Research laboratory has formulated a research problem of the penetration of a labeled tracer antibody in the tumor tissue of a living organism [7]. A system of one-dimensional reactiondiffusion equations
$\frac{\partial u}{\partial t}=\frac{\partial^{2} u}{\partial x^{2}}-k u v, \frac{\partial v}{\partial t}=-k u v$,
which arise from the chemical reaction $A+B \xrightarrow{k} C$, where $A$ is an antibody with a radioactive label, which reacts with substrate $B$, the tissue, affected by the tumor, and $k$ is the reaction rate constant. Concentrations of $A$ and $B$ are denoted by $u$ and $v$, respectively. In deriving equations (11), we assumed that the kinetics of the reaction is described by the mass action law, and reagent $A$ is mobile, whereas reagent $B$ is fixed. We study a semi-infinite plate, inside which substrate $B$ is uniformly distributed. Reagent $A$, when applied to the surface of the plate, begins to penetrate into it. To simulate the penetration of equation (11), in the strip, the following conditions
$S_{T}=\{(x, t): 0<x<\infty, 0<t<T\}$,
with the initial conditions
$u(x, 0)=0, v(x, 0)=v_{0}, x>0$
and the boundary conditions
$u(0, t)=\varphi(t), 0<t<T$,
where $v_{0}$ is a constant - are considered. For the numerical solution, the variable $x$ is converted so that the semi-infinite plate is transformed into the final one. This transformation provides a special family of transformations of Mobius
$\zeta=\frac{x}{x+c}, c>0$.
Each transformation of this family transforms $S_{T}$ into rectangle
$\{(\zeta, t): 0<\zeta<1,0<t<T\}$.
Using $\zeta$, problem (11) is rewritten as
$\frac{\partial u}{\partial t}=\frac{(\zeta-1)^{4}}{c^{2}} \frac{\partial^{2} u}{\partial \zeta^{2}}+\frac{2(\zeta-1)^{3}}{c^{2}} \frac{\partial u}{\partial \zeta}-k u v$,
$\frac{\partial v}{\partial t}=-k u v$,
with initial conditions
$u(\zeta, 0)=0, v(\zeta, 0)=v_{0}, \zeta>0$
and the boundary conditions
$u(0, t)=\varphi(t), \frac{\partial u(1, t)}{\partial \zeta}=0,0<t<T$,
The last boundary condition is obtained from the ratio $\partial u(\infty, t) / \partial x=0$. Discretization of the derivatives in the spatial variables using the method of straight lines leads to the Cauchy problem for a system of ordinary differential equations. For discretization, we used a uniform grid

$$
\left\{\zeta_{i}\right\}, \zeta_{i}=j \cdot \Delta \zeta, \Delta \zeta=\frac{1}{N}, 1 \leq j \leq N
$$

Variables $u_{j}$ and $v_{j}$ denote the approximations $u\left(\zeta_{j}, t\right)$ and $v\left(\zeta_{j}, t\right)$, respectively. It is clear that $u_{j}$ and $v_{j}$ are functions of $t$. The discretizations of the first and second order derivatives on the spatial variable, respectively, have the form
$\frac{\partial u_{j}}{\partial \zeta}=\frac{u_{j+1}-u_{j-1}}{2 \Delta \zeta}$,
$\frac{\partial^{2} u_{j}}{\partial \zeta^{2}}=\frac{u_{j-1}-2 u_{j}+u_{j+1}}{(\Delta \zeta)^{2}}$,
$1 \leq j \leq N$.
The values of $u_{0}$ and $u_{N+1}$, obtained from the boundary conditions, have the form $u_{0}=\varphi(t)$ and $u_{N+1}=u_{N}$. For
$y=\left(u_{1}, v_{1}, u_{2}, v_{2}, \ldots, u_{N}, v_{N}\right)^{T}$
and $T=20$, this semidiscretization problem can be written as
$\frac{d y}{d t}=f(t, y), y(0)=g$,
$y \in R^{2 N}, 0 \leq t \leq 20$,
where $N$ is set by a user parameter. The function $f$ is determined by formulas

$$
\begin{aligned}
f_{2 j-1} & =\alpha_{j} \frac{y_{2 j+1}-y_{2 j-3}}{2 \Delta \zeta} \\
& +\beta_{j} \frac{y_{2 j-3}-2 y_{2 j-1}+y_{2 j+1}}{(\Delta \zeta)^{2}}-k y_{2 j-1} y_{2 j} \\
f_{2 j} & =-k y_{2 j} y_{2 j-1}
\end{aligned}
$$

where
$\alpha_{j}=\frac{2}{c^{2}}(j \Delta \zeta-1)^{3}, \beta_{j}=\frac{1}{c^{2}}(j \Delta \zeta-1)^{4}, 1 \leq j \leq N$,
$\Delta \zeta=\frac{1}{N}, y_{-1}(t)=\varphi(t), y_{2, N+1}=y_{2, N-1}$,
$g \in R^{2 N}, g=\left(0, v_{0}, 0, v_{0}, \ldots, 0, v_{0}\right)^{T}$.
Function $\varphi(t)=2$ for $t \in(0,5]$ and $\varphi(t)=0$ for $t \in(5,20]$, that is, $\varphi$ has a first-order discontinuity at the point $t=5$. According to [7], the appropriate values for the parameters $k, v_{0}$ and $c$ are $k=100, v_{0}=1$ and $c=4$. It also shows the results of calculations with high accuracy and extended bit grating.

The calculations were performed with accuracy $\varepsilon=10^{-4}$. The following calculations were performed with the numerical Jacobi matrix for $N=200$, i.e., system (12) consists of 400 equations. The task of finding the gap of function $\varphi(t)$ at $t=5$ was assigned to the control algorithm of the step. In this paper $i_{f}$ and $i_{j}$ denote, respectively, the total numbers of calculations of the right-hand part and the Jacobi matrix decompositions of the problem (12), which allow to estimate the efficiency of the integration algorithm objectively. The solution of this problem by algorithm was calculated with costs $i_{f}=76717$ and $i_{j}=95$.

## IX. Conclusion

From the above considerations we can draw the following conclusions.

Firstly, stability of $(m, k)$-methods depends on a choice of sets (3), i.e., on a way of implementation of numerical schemes. This follows from a comparison of formulas (8) and (9).

Secondly, a (4,2)-method, which is competitive in accuracy with the implicit method of a Runge-Kutta type with two calculations of the right-hand part of (1) can be constructed. In linear analysis of stability this method is also as good as the implicit method of a Runge-Kutta type. In addition, in (9) a way of implementation is included, i.e., one can estimate computational work per integration step before calculations. Computational work of the implicit methods of a Runge-Kutta type depends highly on a way of implementation. The use of two-stage scheme does not imply that at each step the right-hand part of (1) is calculated twice. Therefore, for some problems the $(4,2)$-method is preferred over implicit numerical formulas of the Runge-Kutta type.

Thirdly, when a function $f(y)$ of problem (1) is calculated twice, an $L$-stable (4,2)-method of the fourth accuracy order can be constructed whereas corresponding L-stable method (2) of the Rosenbrock type can be of order two only. For sufficiently high accuracy of calculations and large dimension of problem (1), decomposition of the Jacobi matrix is responsible, in fact, for total computational work, whereas impact of backward Gauss is unessential. In this case $(4,2)-$ method is more efficient.

Notice, that in the framework of $(m, k)$-methods the problem of freezing the Jacobi matrix can be solved easily [6].

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