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AN ALGORITHM OF VARIABLE STRUCTURE BASED ON THREE-STAGE EXPLICIT-IMPLICIT METHODS

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Abstract. An explicit three-stage Runge-Kutta type scheme and L-stable Rosenbrock method are derived, both schemes of order 3. A numerical formula of order 1 is developed on the base of the stages of the explicit third order method. The stability interval of the first order formula is extended up to 18. The integration algorithm of variable order and step is constructed on the base of these three schemes. For each integration step the most efficient numerical scheme is chosen using an inequality for stability control. Numerical results confirming efficiency of the algorithm are given.

Keywords: stiff problem, one-step method, accuracy and stability control, algorithm of variable structure.

1. Introduction

The Cauchy problem for large-scale stiff systems of ordinary differential equations arises on modelling different processes [1-4]. Numerical schemes of the Rosenbrock type have been widely applied on solving stiff problems lately [5]. These methods can be derived from semi-implicit numerical formulas of the Runge-Kutta type using single iteration in the Newton method. The feature of such methods is that the Jacobi matrix is involved in a numerical formula so to evaluate stages it is enough to solve a linear system several times. The required accuracy is reached via choice of the integration stepsize. Rosenbrock type methods are simple in implementation and their computational costs per step can be easily estimated before calculations.

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However, the introduction of the Jacobi matrix in a numerical formula leads to fundamental problems in case if the same Jacobi matrix is used over several integration steps [6-7]. Note that if the problem to be solved is large-scale, the decomposition of this matrix determines almost all computational costs. Performing calculations with integration algorithms based on explicit and $L-$stable numerical formulas with automatic choice of methods is an alternative to freezing (i.e. using the same matrix over several integration steps) the Jacobi matrix [8-10]. The efficiency of such algorithms is high due to applying explicit methods on transition regions (where derivatives of a solution are large). Choice of the most efficient numerical formula is carried out using an inequality for stability control [3, 11].

Here is formulated the explicit-implicit algorithm of variable structure. The algorithm is based on the $L-$stable Rosenbrock type scheme of order 3 and explicit Runge-Kutta methods of orders 1 and 3. A numerical formula of order 1 is based on stages of the third order explicit method. The stability interval of the first order scheme is extended up to 18. An integration algorithm of alternating order and step is formulated. Choice of the most efficient numerical scheme is performed at each step applying an inequality for stability control. Numerical results confirming efficiency of the algorithms are given.

2. EXPLICIT THIRD ORDER METHOD

The Cauchy problem for a system of differential equations

$$y' = f(y),\ y(t_0) = y_0,\ t_0 \le t \le t_k, \tag{1}$$

is considered, where y and f are real N-dimensional vector-functions, t is an independent variable. To solve (1) the following explicit three-stage method of the Runge-Kutta type

$$\begin{gathered} y_{n+1} = y_n + p_1 k_1 + p_2 k_2 + p_3 k_3, \\ k_1 = hf(y_n),\ k_2 = hf(y_n + \beta_{21} k_1), \\ k_3 = hf(y_n + \beta_{31} k_1 + \beta_{32} k_2), \end{gathered} \tag{2}$$

is applied, where h represents the integration stepsize, k_1, k_2, and k_3 are stages of the method, $p_1, p_2, p_3, \beta_{21}, \beta_{31}$, and β_{32} are numerical coefficients defining accuracy and stability properties of (2). For a nonautonomous system

$$y' = f(t, y),\ y(t_0) = y_0,\ t_0 \le t \le t_k,$$

numerical formula (2) takes the form

$$\begin{gathered} y_{n+1} = y_n + p_1 k_1 + p_2 k_2 + p_3 k_3, \\ k_1 = hf(t_n, y_n),\ k_2 = hf(t_n + \beta_{21} h, y_n + \beta_{21} k_1), \\ k_3 = hf(t_n + [\beta_{31} + \beta_{32}]h, y_n + \beta_{31} k_1 + \beta_{32} k_2). \end{gathered}$$

For simplicity, hereinafter we consider problem (1). However, all the derived methods can be applied to nonautonomous problems. Let us use here the third order method developed in [12]. For that, let $\beta_{21} = 0.5$ and $\beta_{31} + \beta_{32} = 1$. Then, at each step increments k_1, k_2, and k_3 are computed at points t_n, $t_n + 0.5h$, and $t_n + h$, respectively. The uniform distribution of points provides higher reliability of calculations. In this case coefficients of the third order method are

$$\beta_{21} = \frac{1}{2},\ \beta_{31} = -1,\ \beta_{32} = 2,\ p_1 = \frac{1}{6},\ p_2 = \frac{2}{3},\ p_3 = \frac{1}{6}, \tag{3}$$

and its local truncation error $\delta_{n,3}$ has the form

$$\delta_{n,3} = \frac{1}{24}h^4\Big[f'^3 f - f''f'f^2 - \frac{1}{3}f'''f^3\Big] + O\big(h^5\big).$$

The inequality for accuracy control of method (2), (3) is obtained using the idea of embedded methods and takes the form [12]

$$\frac{1}{6}\cdot\big\|k_1 - 2k_2 + k_3\big\| \le \varepsilon,$$

where $\|\cdot\|$ denotes some norm in R^N, ε is the defined tolerance of calculations.

The inequality for stability control of numerical formula (2) is derived using the approach offered in [3, 11]. The estimate $v_{n,3} = h\cdot\lambda_{n,\max}$ for the maximum eigenvalue of the Jacobi matrix of problem (1) is evaluated using power iterations through stages that have been already computed. As a result, it is given by the formula [12]

$$v_{n,3} = 0.5\max_{1\le i\le N}\Big|\frac{k_1^i - 2k_2^i + k_3^i}{k_2^i - k_1^i}\Big|. \tag{4}$$

Stability interval of scheme (2), (3) approximately equals 2.5. Therefore, for its stability control we can apply inequality $v_{n,3} \le 2.5$.

3. FIRST ORDER METHOD

Now, let us apply to problem (1) the following scheme

$$\begin{gathered} y_{n+1} = y_n + r_1k_1 + r_2k_2 + r_3k_3,\\ k_1 = hf\big(y_n\big),\ k_2 = hf\big(y_n + \beta_{21}k_1\big),\\ k_3 = hf\big(y_n + \beta_{31}k_1 + \beta_{32}k_2\big), \end{gathered} \tag{5}$$

where coefficients β_{21}, β_{31}, and β_{32} have been already defined when deriving the third order method, whereas r_1, r_2, and r_3 are to be obtained. According to [12] we have the coefficients

$$r_1 = \frac{673}{729},\ r_2 = \frac{52}{729},\ r_3 = \frac{4}{729}$$

of the first order method with maximal stability interval, which local truncation error $\delta_{n,1}$ can be written as follows

$$\delta_{n,1} = \frac{19}{54}h^2 f'f + O(h^3).$$

To control accuracy of the first order numerical formula we use local error estimate. Taking into account the form of local error $\delta_{n,1}$ and allowing for

$$k_2 - k_1 = 0.5h^2 f_n' f_n + O(h^3)$$

we can write the inequality for accuracy control in the form

$$\frac{19}{27}\cdot\big\|k_2 - k_1\big\|\le \varepsilon,$$

where $\|\cdot\|$ denotes some norm in R^N, ε is the defined tolerance of calculations. Stability interval of numerical scheme (5) of the first order equals 18 [3]. Hence, for its stability control inequality $v_{n,3} \le 18$ can be applied, where $v_{n,3}$ is given by formula (4).

4. ROSENBROCK TYPE METHOD

Now to solve problem (1) consider numerical formula of the form

$$y_{n+1} = y_n + p_1 k_1 + p_2 k_2 + p_3 k_3,\ D_n = E - ahf'_n,$$
$$D_n k_1 = hf\big(y_n\big),\ D_n k_2 = hf\big(y_n + \beta_{21} k_1\big), \tag{6}$$
$$D_n k_3 = hf\big(y_n + \beta_{31} k_1 + \beta_{32} k_2\big),$$

where h represents stepsize, E is the identity matrix, $f'_n = \partial f\big(y_n\big)/\partial y$ is the Jacobi matrix of system (1), a, p_i, and β_{ij} are numerical coefficients. Comparing the Taylor series for exact and approximate solutions up to terms with h^3, get the third order conditions for scheme (6):

$$p_1 + p_2 + p_3 = 1,\ \beta_{21} p_2 + \big(\beta_{31} + \beta_{32}\big) p_3 = \frac{1}{2} - a,$$
$$\beta_{21}^2 p_2 + \big(\beta_{31} + \beta_{32}\big)^2 p_3 = \frac{1}{3}, \tag{7}$$
$$\beta_{21} \beta_{32} p_3 = \frac{1}{6} - a + a^2.$$

Let us study stability of numerical formula (6). Applying it to the test Dahlquist equation $y' = \lambda y$ [13], we have $y_{n+1} = Q_{roz}(x) y_n$, where λ represents some eigenvalue of the Jacobi matrix of problem (1), $x = h \cdot \lambda$. The stability function $Q_{roz}(x)$ under conditions (7) takes the form

$$Q_{roz}(x) = \frac{1 + \big(1 - 3a\big)x + \big(3a^2 - 3a + 0.5\big)x^2}{\big(1 - ax\big)^3} -$$
$$- \frac{\big(a^3 - 3a^2 + 1.5a - 1/6\big)x^3}{\big(1 - ax\big)^3}.$$

The necessary condition providing L-stability of numerical formula (6) implies that degree of the polynomial staying in numerator of $Q_{roz}(x)$ be less than degree of the polynomial in denominator. It is easy to see that this requirement is satisfied if the following relation is true

$$a^3 - 3a^2 + \frac{3}{2}a - \frac{1}{6} = 0.$$

The given equation has three real roots

$$a_1 = 2.40514957850286,\ a_2 = 0.158983899988677,\ a_3 = 0.435866521508459,$$

computed by the dichotomy method. According to [14] scheme (6) is $A-$stable, if parameter a satisfies the inequalities $0.(3) \le a \le 1.0685790$. As a result, hereinafter we assume that $a = 0.435866521508459$. In this case scheme (6) is $L-$stable.

Uniform distribution of points over interval $[t_n, t_{n+1}]$ in a number of instances provides higher reliability of calculations [15]. Let $\beta_{21} = 0.5$ and $\beta_{31} + \beta_{32} = 1$. Then, k_1, k_2, and k_3 are computed at points t_n, $t_n + 0.5h$, and $t_n + h$, respectively. As a result, coefficients of (6) are of the form

$$a = 0.435866521508459,\ p_1 = 3a + \frac{1}{6},$$
$$p_2 = \frac{2}{3} - 4a,\ p_3 = a + \frac{1}{6},\ \beta_{21} = \frac{1}{2}, \tag{8}$$

$$\beta_{31} = -\frac{12a^2 - 18a + 1}{6a + 1}, \ \beta_{32} = \frac{12a^2 - 12a + 2}{6a + 1}.$$

To control accuracy of calculations and choose the stepsize automatically we use here an embedded method. On solving stiff problems with the third order methods error behaviour is determined by main member $h^4 f'^3 f$ of local error [3]. Thus, in derivation of the error estimate we allow for only the first summand in the local error:

$$\delta_{n,3}^{roz} = \frac{1 - 12a + 36a^2 - 24a^3}{24} h^4 f'^3 f + O\big(h^4\big).$$

To get an inequality for accuracy control of calculations let us consider 2-stage method

$$y_{n+1,2} = y_n + b_1 k_1 + b_2 k_2, \tag{9}$$

where y_n is computed by formula (6). Note that numerical formula (9) uses stages of method (6), and, hence, applying (9) leads to almost no increase in computational costs. Expanding stages in the Taylor series it is easy to see that on coefficients $b_1 = 2a$ and $b_2 = 1 - 2a$ scheme (9) is order 2 and its local error $\delta_{n,2}$ is of the form

$$\delta_{n,2} = \frac{6a^2 - 6a + 1}{6} h^3 f'^2 f + O\big(h^3\big).$$

Allowing for the forms of $\delta_{n,2}$ and $\delta_{n,3}$ in the inequality for accuracy control the following error estimate [16]

$$\varepsilon\big(j_n\big) = \frac{1 - 12a + 36a^2 - 24a^3}{4\big(6a^2 - 6a + 1\big)} D_n^{1-j_n}\big(y_{n+1} - y_{n+1,2}\big).$$

can be applied. On $j_n = 1$ estimate $\varepsilon\big(j_n\big)$ is $A-$stable, whereas on $j_n = 2$ it is $L-$stable. Now, the inequality for accuracy control takes the form

$$\Big\| D_n^{1-j_n}\big(y_{n+1} - y_{n+1,2}\big)\Big\| \le c \cdot \varepsilon, \ 1 \le j_n \le 2, \tag{10}$$

where

$$c = 4 \cdot \left| \frac{6a^2 - 6a + 1}{1 - 12a + 36a^2 - 24a^3} \right| \approx 3,$$

$\| \cdot \|$ denotes some norm in R^N, ε is the defined tolerance, and parameter j_n is taken smallest for which inequality (10) is satisfied. Note that in terms of the main member estimates $\varepsilon(1)$ and $\varepsilon(2)$ are equivalent. Inequality (10) is seldom checked on $j_n = 2$, usually it happens if the integration stepsize changes dramatically. The additional check of $\varepsilon(2)$ allows to avoid unnecessary returns (recomputations of a solution) arising due to the wrong asymptotic behaviour of error estimate $\varepsilon(1)$.

5. INTEGRATION ALGORITHM OF VARIABLE STRUCTURE

It is not difficult to formulate an algorithm of variable order and step on the base of the derived above explicit methods of orders 1 and 3. Calculations are always started with the third order method as it is more accurate. Transition to the first order scheme is performed on violation of inequality $v_{n,3} \le 2.5$. Return to the third order method is done if inequality $v_{n,3} \le 2.5$ is satisfied. On calculations with the first order method stability is controlled along with accuracy, and predicted step h_{n+1} is given by the formula

$$h_{n+1} = \max\Big[h_n, \min\big(h^{ac}, h^{st}\big)\Big],$$

where h_n represents last successful stepsize, h^{ac} and h^{st} are stepsizes chosen according to the accuracy and stability requirements, respectively. Note that this formula is used to predict integration stepsize h_{n+1} after successful computation of a solution with previous stepsize h_n, and, hence, gives almost no increase in computational costs. In the same time such a way of choosing stepsize limits its value over the settling region and does not let it oscillate. Notice that it is existence of settling regions that limits application of explicit methods to stiff problems.

In case of using scheme (6) formulation of the integration algorithm also does not cause difficulties. Violation of $v_{n,3} \le 18$ causes transition from the explicit first order method to $L-$stable numerical scheme (6). Explicit methods work when inequality $v_{n,0} \le 18$ is satisfied, where estimate $v_{n,0} = h\lambda_{n,\ \max}$ of the maximum eigenvalue of the Jacobi matrix of system (1), necessary for transition to the explicit formulas is computed through the Jacobi matrix norm

$$v_{n,0} = h \cdot \Big|\frac{\partial f(y_n)}{\partial y}\Big| = h \cdot \max_{1\le i\le N} \left\{ \sum_{j=1}^{N} \Big|\frac{\partial f_i(y_n)}{\partial y_j}\Big| \right\}.$$

Norm $\|\varphi\|$ in inequalities for accuracy control is evaluated by the formula

$$||\varphi|| = \max_{1\le i\le N} \left\{ \frac{|\varphi_i|}{|y_n^i| + r} \right\},$$

where i represents the component number, r is a positive parameter. If in i-th component of a solution inequality $|y_n^i| < r$ is satisfied, then absolute error $r\varepsilon$ is controlled, otherwise – relative error ε.

On numerical evaluation of the Jacobi matrix its $j-$th column has the form

$$\frac{\partial f}{\partial y_j} = \frac{f\big(y_1, \cdots, y_j + r_j, \cdots, y_N\big) - f\big(y_1, \cdots, y_j, \cdots, y_N\big)}{r_j}.$$

In calculations numerical differentiation step r_j is chosen using the formula

$$r_j = \max\big(10^{-14}, 10^{-7}|y_j|\big).$$

Calculations are assumed to be performed with double precision. Constant 10^{-7} is introduced to put the step of numerical differentiation in the middle of bit grid.

6. NUMERICAL RESULTS

Calculations were performed on PC Intel(R) Core i5-3317U CPU@1.70GHz with double precision. On computation of the error norm parameter r was set to 1 so that relative and absolute tolerances were equal. Calculations were performed with the defined tolerance $\varepsilon = 10^{-4}$ and $\varepsilon = 10^{-6}$. In latter case over sufficient long region of the integration interval the stepsize is limited according to the accuracy requirements. This allows to see the advantage of the explicit-implicit algorithm more clearly. If the accuracy of calculations is low for some problems the number of switches on the explicit methods may be small or they may be absent. It usually happens when stepsize is limited according to the stability requirements all the time. On calculations with the $L-$stable Rosenbrock type method for all the test problems calculations were performed with the numerical Jacobi matrix.

The first test problem is the Van-der-Pol oscillator [17]

$$y_1' = y_2,\ y_2' = \mu\Big[\big(1 - y_1^2\big)y_2 - y_1\Big],$$

$$t \in [0, 10],\ y_1(0) = 2,\ y_2(0) = 0.$$

The feature of this example is significant number of alternating transition and settling regions. On such problems the maximum efficiency of the combined integration algorithms is supposed. Numerical results for the Van-der-Pol problem are given in the Tables 1 and 2.

Table 1. Numerical results for the Van der Pol problem, $\varepsilon = 10^{-4}$, $\mu = 10^2$

Solver	**Steps**	**Eval. Stages**	**Returns**	**Num. Jac**	**Decs**
Variable structure algorithm	3266	12057	1101	864	921
Explicit algorithm	9046	29194	1028	0	0
L-stable Rosenbrock method	1387	5328	389	1387	1776

Table 2. Numerical results for the Van der Pol problem, $\varepsilon = 10^{-6}$, $\mu = 10^3$

Solver	**Steps**	**Eval. Stages**	**Returns**	**Num. Jac**	**Decs**
Variable structure algorithm	26948	94322	6739	5962	5962
Explicit algorithm	146436	448034	4363	0	0
L-stable Rosenbrock method	11522	37080	838	11522	12360

It follows from the numerical results for the first problem that the derived algorithm has 1.5-2 times less decompositions of the Jacobi matrix comparing to the L-stable Rosenbrock scheme. It means that new algorithm is preferable on solving large-scale problems of low and moderate stiffness. Note that the variable structure algorithm is less accurate than just the L-stable Rosenbrock method due to the use of the first order method in former. Numerical results for the explicit algorithm are given to show possibility of applying explicit methods with extended stability domains to rather stiff problems.

The following example is described by 2 differential equations in partial derivatives with initial and boundary conditions. The Akzo Nobel research laboratory formulated this problem in their study of the penetration of radio-labeled antibodies into a tissue that has been infected by a tumor [18]. There is considered a reaction diffusion system in one spatial dimension:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - kuv,\ \frac{\partial v}{\partial t} = -kuv \tag{11}$$

which originates from the chemical reaction $A + B \xrightarrow{k} C$, here A is the radio-labeled antibody, reacts with substrate B, the tissue with the tumor, and k denotes the rate constant. The concentrations of A and B are represented by u and v, respectively.

Making necessary transformations and defining $y(t)$ by $y = (u_1, v_1, u_2, v_2, ..., \ u_N, v_N)^T$ it is possible to write (11) in the form

$$\frac{dy}{dt} = f(t, y), \quad y(0) = g, \quad y \in R^{2N}, \quad 0 \le t \le 20.$$

Here N is a user-supplied parameter. The function f is given by

$$f_{2j-1} = \alpha_j \frac{y_{2j+1} - y_{2j-3}}{2\triangle\zeta} + \beta_j \frac{y_{2j-3} - 2y_{2j-1} + y_{2j+1}}{(\triangle\zeta)^2} - k y_{2j-1} y_{2j},$$

$$f_{2j} = -k y_{2j} y_{2j-1},$$

where

$$\alpha_j = \frac{2(j\Delta\zeta - 1)^3}{c^2}, \ \beta_j = \frac{(j\Delta\zeta - 1)^4}{c^2}, \ 1 \le j \le N,$$

$$\Delta\zeta = \frac{1}{N}, \ y_{-1}(t) = \varphi(t), \ y_{2,N+1} = y_{2,N-1},$$

$$g \in \mathbb{R}^{2N}, \ g = (0, v_0, 0, v_0, \ \ldots, 0, v_0)^{\mathrm{T}}.$$

Function $\varphi(t) = 2$ for $t \in (0, 5]$ and $\varphi(t) = 0$ for t $\in (5, 20]$, i.e. φ undergoes a discontinuity in time at $t = 5$. Calculations were performed with parameters $k = 100$, $v_0 = 1$, and $c = 4$. Numerical results obtained with high accuracy and with double precision are given in [18].

Calculations were performed on $N = 200$, i.e. the corresponding system involved 400 ordinary differential equations. The problem of finding discontinuity of $\varphi(t)$ at $t = 5$ was solved by the stepsize control algorithm.

Table 3. Numerical results for the Medical Akzo Nobel Problem, $\varepsilon = 10^{-4}$

Solver	**Steps**	**Eval. Stages**	**Returns**	**Num. Jac**	**Decs**
Variable structure algorithm	575	2125	176	413	461
L-stable Rosenbrock method	364	1206	38	364	402

The second test problem is too stiff for new algorithm. Numerical results for the second problem show degradation of the efficiency.

On solving both test examples there is plenty of declined solutions arising on applying explicit methods. The solution to this problem is designing similar algorithm involving an explicit scheme with wider stability interval (and probably higher accuracy order). Further gain in the efficiency can be provided via using economical procedures for evaluation and decomposition of the Jacobi matrix.

7. CONCLUSION

The derived explicit-implicit algorithm is aimed at solving large-scale problems of moderate stiffness with low accuracy. In this case it is most efficient. In the algorithm via its parameters it is possible to specify different modes of calculations with: 1) the explicit first order and third order methods either with or without stability control; 2) explicit methods of alternating order and step; 3) the L-stable method using either analytical or numerical Jacobi matrix; 4) automatic choice of a numerical scheme. Therefore, this algorithm can be applied to stiff as well as non-stiff problems. In calculations with automatic choice of a numerical scheme, the integration algorithm makes a decision whether a problem to be solved is stiff or not by itself. All the methods involved in the explicit-implicit algorithm are implemented separately, controlled by a single program and can be easily withdrawn. This allows performing numerical experiments on a specific class of problems in order to find the most efficient algorithm from the given set with its subsequent disengagement.

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