Explicit-Implicit Variable Structure Algorithm for Solving Stiff Systems

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Abstract—An algorithm of variable structure for solving stiff problems is constructed using L-stable and explicit methods. It is based on explicit and L-stable methods, both schemes of order two, and on an explicit method of the first order, which interval of stability is extended. On each step an efficient numerical scheme is chosen by criterion of stability. The numerical results of modeling the simplest oregonator and the modified oregonator exhibiting complicated limit cycle are given.

Keywords—Stiff system, accuracy and stability control, variable structure algorithms.

I. INTRODUCTION

The Cauchy problem for stiff systems of ODEs arises in many applications [1, 2]. The main trends in construction of numerical methods are associated with expansion of their possibilities in solving large-scale problems.

In many cases calculations are required to be conducted within limits of so called engineering accuracy about 1% and lower. This is due to the fact, that measurement of constants in a right part of a system of differential equations is often quite rough. Sometimes, such accuracy of calculations is satisfactory in terms of a goal. It is well-known (see, e.g. [3]), that order of approximation of a numerical scheme should be associated with required accuracy of calculations. Therefore, below we shall consider only those numerical formulas, that have order of accuracy less or equal to two.

Modern methods for solving stiff problems usually use calculation and inversion of the Jacobi matrix of a system of differential equations. In case of a sufficiently large dimension, efficiency of numerical methods is almost completely determined by inversion (decomposition) of the matrix. To increase efficiency of calculations in a number of algorithms, the freezing of the Jacobi matrix is used, that means using same matrix on several steps of integration [4]. This approach is the most successful in algorithms based on multistep methods and, in particular, in backward differentiation formulas [5]. This problem does not cause any particular difficulties in constructing integration algorithms based on other numerical schemes, if their stages are computed with the Jacobian matrix in some iterative process.

This is due to the fact, that in this case the Jacobian matrix does not affect accuracy order of a numerical scheme, but only determines rate of convergence of iterations. So, it needs to be recomputed, when there is a significant slowdown on convergence rate of the iterative process.

The situation is worse in an integration algorithm, based on known noniterative methods, which include methods of the Rosenbrock type [6] and their various modifications [4]. It should be noted, that the noniterative method is much simpler in terms of computer implementation than algorithms, based on numerical formulas, which are evaluated with using iterations. However, in methods of form [6], the Jacobi matrix affects accuracy order of a numerical scheme and, therefore, difficulties with its freezing arise. If a problem of using same matrix on several steps of integration is left unsolved, then, obviously one is limited to solve only problems of low dimensions. In [7, 8], this problem is considered in relation to the Rosenbrock methods. It is proved, that maximum accuracy order of the Rosenbrock methods is equal to two, if in an integration algorithm the same Jacobi matrix is applied on several steps of integration. There is an algorithm with freezing the Jacobi matrix, based on L-stable numerical formulas of second accuracy order and results of calculations, confirming its high efficiency.

Another important requirement for modern integration algorithms is numerical approximation of the Jacobi matrix. This is due to the fact, that a right part of a system of differential equations often has large dimensions and quite complex form. A typical example is provided by problems of chemical kinetics, where complexity of a right part increases with number of elementary stages in a chemical reaction. Nowadays, simulation involves reactions, which contain dozens of reagents and hundreds of elementary stages. Therefore, in some cases, less effective numerical methods are more preferable, if their implementation does not require the analytical calculation of elements of the Jacobi matrix. This barrier can be removed if an integration algorithm includes possibility of numerical approximation of the Jacobi matrix. Note, that the problems of freezing and numerical approximation are in some sense close to each other and, therefore, can be solved simultaneously.

Some analog of freezing the Jacobi matrix is using in calculations integration algorithms, based on explicit and L-stable methods with automatic selection of a numerical scheme. In this case, efficiency of the algorithm can be

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improved by calculating transitive regions corresponding to a
maximum eigenvalue of the Jacobi matrix by an explicit
method. It is natural to apply an inequality for stability control
[9] as a criterion for choosing an efficient numerical formula.
Note, that using such hybrid algorithms does not fully
eliminate the problem of freezing the Jacobi matrix, because
the explicit method can be applied, generally speaking, only
for a boundary layer solution, corresponding to a maximum
eigenvalue of the Jacobi matrix.

Here, based on the explicit methods of the Runge-Kutta type
of the first and second orders, as well as the L-stable (2,1)-
method of second-order accuracy, an algorithm of variable
structure is constructed, which allows both a numerical and an
analytical Jacobi matrix. Numerical results confirm high
efficiency of the integration algorithm.

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II. L-STABLE (2,1)-METHOD

In [10] for numerical solution of the Cauchy problem for
stiff systems of ordinary differential equations
\[ y' = f(t, y), \quad y(t_0) = y_0, \quad t_0 \leq t \leq t_1, \]
(1)
where \( y \) and \( f \) are real \( N \)-dimensional vector functions, \( t \)
is an independent variable, the class of \((m,k)\)-methods is
proposed. From the standpoint of computer implementation,
\((m,k)\)-methods are as simple as the Rosenbrock schemes.
However, in contrast to the Rosenbrock methods, in this class
it is much easier to solve a problem of freezing the Jacobi
matrix and its numerical approximation. In addition, \((m,k)\)-
methods have more good properties of accuracy and stability
with slight increase of computational cost. In traditional
methods, number of stages \( m \) completely describes a
numerical formula. In \((m,k)\)-methods two constants are
required to describe numerical schemes: number of stages \( m \)
and number of calculations of a right part of the system (1)
on an integration step \( k \).

To solve the problem (1), we consider a (2,1)-scheme
\[ y_{n+1} = y_n + p_1 k_1 + p_2 k_2, \]
(2)
where \( k_1 \) and \( k_2 \) are stages of the method; \( D_n = E - a_0 A_n \), \( E \)
is an identity matrix, \( h \) is an integration step, \( A_n \) is some
matrix, which can be represented in a following form
\[ A_n = f_n + hB_n + O(h^2), \]
(3)
where \( f_n = \frac{\partial f}{\partial y}(t_n, y_n) \) is the Jacobi matrix of the system (1), \( B_n \)
is an independent of an integration step arbitrary matrix, \( a \),
\( \beta \), \( p_1 \) and \( p_2 \) are numerical coefficients. Using the matrix \( A_n \)
represented in form (3) allows us to apply (2) with freezing
both an analytical and a numerical Jacobi matrix [11]. In case
of using the Jacobi matrix \( f_n \), calculated \( k \) steps back we have
\[ B_n = -h^2 f_n, \quad f^2 f_n = \frac{\partial^2 f}{\partial y^2}(y_n) \]
If the Jacobi matrix is computed numerically with a step
\( r_j = c/h \), then elements \( b_{n,j} \) of the matrix \( B_n \) have a form
\[ b_{n,j} = 0.5c \Delta^2 f,(t_n, y_n) / \Delta^2 y \] .
In calculations the step \( r_j \) is chosen according to a formula
\[ r_j = \max(10^{-14}, 10^{-7} | y_j |) . \]

Let’s obtain the coefficients of the \( L \)-stable numerical
scheme (2) of second order and an inequality for accuracy
control. An expansion of an exact solution \( y(t_n) \) in the
Taylor series in a vicinity of a point \( t_n \) to terms with \( h^3 \)
inclusive has a form
\[ y(t_{n+1}) = y(t_n) + hf + \frac{1}{2} h^2 \left[ f'_n + f'_{n+1} \right] + \frac{1}{6} h^3 \left[ f''_n + f''_{n+1} + 2f'_n f''_n + f''_{n+1} f'_{n+1} + f''_{n+1} f''_{n+1} \right] + O(h^4) \]
(4)
where the elementary differentials are calculated on an
exact solution \( y(t_n) \). To find the coefficients \( \beta, a, p_1 \) and \( p_2 \) of
the scheme (2) we write an expansion of the stages \( k_1 \) and \( k_2 \) in a
Taylor series in a vicinity of a point \( y_n \) to terms with \( h^2 \)
inclusive and substitute it in (2). We obtain
\[ y_{n+1} = y_n + \left( p_1 + p_2 \right) h f_n + \beta \left( p_1 + p_2 \right) h^2 f'_{n+1} \]
\[ + a \left( p_1 + 2p_2 \right) h^2 f''_n f_n + \frac{1}{2} \beta^2 \left( p_1 + p_2 \right) h^3 f''_{n+1} \]
\[ + a \beta \left( p_1 + 2p_2 \right) h^2 f'_n f'_{n+1} + a^2 \left( p_1 + 3p_2 \right) h^3 f''_{n+1} f_n + \]
\[ + a \left( p_1 + 2p_2 \right) h^2 B_n f_n + O(h^4) \]
(5)
where the elementary differentials are calculated on an
approximate solution \( y_n \). Assuming, that \( y_n = y(t_n) \) and
comparing the expansions (4) and (5) to terms with \( h^3 \)
inclusive, we obtain conditions of second-order accuracy of
scheme (2), i.e.
\[ p_1 + 2p_2 = 1, \quad a(p_1 + 2p_2) = \frac{1}{2}, \quad \beta = \frac{1}{2} \]
(6)

Let’s investigate stability of a numerical formula (2). Applying it to a problem
\[ y' = \lambda y, \quad y(0) = y_0, \quad \text{Re}(\lambda) < 0, \]
(7)
we obtain \( y_{n+1} = Q(x)y_n, x = h\lambda \), where a function of stability
\( Q(x) \) has the following form
\[ Q(x) = 1 + \frac{1}{2}(p_1 + 2p_2 - 2a)x + a(a - p_1)x^2 \]
\[ - \frac{1}{2} \left(1-ax^2 \right) \] .
Then, the scheme (2) is \( L \)-stable, if \( p_1 = a \). Substituting this
relation in (6), we obtain a set of the coefficients
\[ p_1 = a, \quad p_2 = 1 - a, \quad \beta = \frac{1}{2} \]
(8)
where \( a \) is determined from a \( L \)-stability condition
\[ a^2 - 2a + \frac{1}{2} = 0 \] .
(9)
Comparing (4) and (5) to terms with \( h^3 \) inclusive, we find,
that a local error \( \delta_n \) of the numerical scheme (2) with the
coefficients (8) have a form
\[ \delta_n = \left( a - \frac{1}{3} \right) h^3 f''^2 f + \frac{1}{2 h} f''^2 + \frac{1}{6} h f''^2 f^2 \\
+ \frac{1}{3} h f'' f^2 - \frac{1}{2} h f' f + \frac{1}{6} B_n f + O(h^4). \] (10)

The equation (9) has two roots \( a_i = 1 - 0.5\sqrt{2} \) and \( a_i = 1 + 0.5\sqrt{2} \). We choose \( a = a_1 \), as in this case the coefficient in the leading term \((a-1/3)h^3f''^2f\) of error (10) is less.

Let's consider simultaneously the numerical Rosenbrock formula with two calculations of the function \( f \) on each step

\[ y_{n+1} = y_n + p_1 k_1 + p_2 k_2, \]
\[ D_1 k_1 = hf(y_n), \quad D_2 k_2 = hf(y_n + a k_1). \] (11)

According to [7], for \( \gamma = a \), a set of coefficients (8) provides a second accuracy order of (11), and condition (9) provides its L-stability. It follows from [7] that the numerical formula (11) with the coefficients (8) is one of the most efficient among the methods of the Rosenbrock type, with two computations of a right part of a differential problem on an integration step. A local error \( \delta^\text{loc} \) of the numerical formula (11) has a form

\[ \delta^\text{loc}_n = h^3 \left[ a - \frac{1}{3} \right] f''^2 f + \frac{1}{6} h f''^2 f^2 \\
- ah^3 B_n f + O(h^4). \] (12)

The scheme (2) with coefficients (8) as well as scheme (11) with coefficients (8) has a second accuracy order and L-stability, and their local errors (10) and (12) differ slightly. At the same time, the scheme (2) requires one less calculation of function \( f \) than (11) on each step, with other costs being equal, which makes it more preferable.

We construct accuracy control of the numerical scheme (2) by analogy with [12]. For this purpose, we denote

\[ \nu(j_n) = D_n^{-1} k_2 - k_1, \] (13)

where \( k_1 \) and \( k_2 \) are calculated by the formulas (2). Then, according to [12], in order to control the accuracy on each step, one has to control an inequality

\[ \left\| \nu(j_n) \right\| \leq \varepsilon, \quad 1 \leq j_n \leq 2, \] (14)

where \( \varepsilon \) is required accuracy of calculations, \( \| \| \) is some norm in \( \mathbb{R}^n \), and the integer variable \( j_n \) is selected as the lowest, for which inequality (14) holds.

Note one important feature of error estimation (13). The scheme (2) is L-stable, that is, for its stability function \( Q(x) \), the relation \( Q(x) \to 0 \) for \( x \to -\infty \) holds. Since for an exact solution \( y(t_{n+1}) = \exp(x)y(t_n) \) of the problem (7) a similar property holds, it is natural to require convergence to zero of the error estimation for \( x \to -\infty \). However, for \( \nu(1) \) this property is not satisfied — this estimation has an A-stable manner.

To correct asymptotic behavior of the estimated error we introduced an estimation \( \nu(j), 1 \leq j \leq 2 \) instead of \( \nu(1) \). In this case, behavior of error estimations for \( j_n = 2 \) will be coordinated with behavior of the exact solution of the test problem for \( x \to -\infty \). We emphasize, that in sense of a general member, estimations \( \nu(1) \) and \( \nu(2) \) coincide. Using \( \nu(j_n) \) actually does not lead to increase of computational costs. This is due to the fact, that \( \nu(j_n) \) for \( j_n = 2 \) is checked only when it is violated for \( j_n = 1 \). This situation appears rarely, mainly when an integration step grows rapidly. However, this allows us to choose the step more accurately and thereby reduce the number of unnecessary recomputing solutions (returns).

An estimation of a maximum eigenvalue \( w_{n,0} = h\lambda_{n,\max} \) of the Jacobi matrix of the system (1), necessary to switch to an explicit formula, is estimated through its norm \( w_{n,0} = h\|\partial f(t_n, y_n)/\partial y\| \). Below, this estimation will be used for automatic selection of a numerical scheme.

III. EXPLICIT SECOND ORDER RUNGE-KUTTA METHOD

For solution the problem (1) we consider an explicit two-stage Runge-Kutta method [13]

\[ y_{n+1} = y_n + p_1 k_1 + p_2 k_2, \]
\[ k_1 = hf(y_n), \quad k_2 = hf(y_n + \beta k_1). \] (15)

Let's consider the autonomous problem (1) to simplify formulas. In case of a non-autonomous system \( y' = f(t, y) \) the scheme (15) is written as

\[ y_{n+1} = y_n + p_1 k_1 + p_2 k_2, \]
\[ k_1 = hf(t_n, y_n), \quad k_2 = hf(t_n + \beta h, y_n + \beta k_1). \]

We obtain relations for the coefficients of the method (15) of second accuracy order. For this purpose, we expand the stages \( k_1 \) and \( k_2 \) in Taylor series in powers of \( h \) up to terms with \( h^2 \) inclusive, and substitute them in the first formula (15). As a result, we obtain

\[ y_{n+1} = y_n + (p_1 + p_2) hf' + \beta p_1 h^2 f' f_n \\
+ \frac{1}{2} \beta^2 h^3 p_2 f'' f_n^2 + O(h^4), \]

where the elementary differentials are calculated on the approximate solution \( y_n \). Comparing this expression with (4) to terms with \( h^2 \) inclusive, assuming, that \( y_n = y(t_n) \), we write conditions \( p_1 + p_2 = 1 \) and \( \beta p_2 = 0.5 \) of second accuracy order of the scheme (15). In these relations, the local error \( \delta_n \) of the scheme (15) can be written as follows

\[ \delta_n = h^3 \left[ \frac{1}{6} f''^2 f + \frac{2 - 3\beta}{12} f' f^2 \right] + O(h^4). \]

We construct an inequality for accuracy control. For this purpose, we consider an auxiliary scheme \( y_{n+1,1} = y_n + k_1 \) of first accuracy order. Using the idea of nested methods, estimation of error \( \delta_{1,2} \) of the second-order method can be calculated by formula [12]
\[ e_{n,2} = y_{n+1} - y_{n+1,1} = p_1(k_1 - k_2). \]

To improve reliability of this estimation, we choose \( \beta = 1 \).

Then, stage \( k_1 \) is computed at the point \( t_n \), and \( k_2 \) is computed at the point \( t_{n+1} \). Calculations show, that using information in extreme points of a step leads to more reliability. For \( \beta = 1 \), coefficients of the method of second order are uniquely determined \( p_1 = p_2 = 0.5 \) and a local error and an accuracy control inequality are, respectively, given below
\[
\delta_n = \frac{h^3}{12} \left[ 2f'(f - f') \right] + O(h^4), \quad 0.5\|k_2 - k_1\| \leq \varepsilon.
\]

Now, we construct an inequality for stability control of (15) by method proposed in [9]. For this purpose, we consider an auxiliary stage \( k_1 = hf(y_{n+1}) \). Note, that \( k_i \) coincides with the stage \( k_i \), which is used on a next integration step and, therefore, its applying does not lead to additional computing of the right part of (1). We write the stages \( k_1 \), \( k_2 \) and \( k_3 \) to a problem \( y' = Ay \), where \( A \) is a matrix with constant coefficients. A result is given below
\[
k_i = Xy_n, \quad k_2 = (X + X^2)y_n, \quad k_3 = (X + X^2 + 0.5X^3)y_n,
\]

where \( X = hA \). It is easy to see, that
\[
k_2 - k_1 = Xy_n, \quad 2(k_3 - k_2) = X^2y_n.
\]

Then, according to [9] an estimation of a maximum eigenvalue \( w_{n,2} = h\lambda_{-\text{max}} \) of the Jacobi matrix of the system (1) can be calculated by a following formula
\[
w_{n,2} = 2\max_{1 \leq i \leq N} \left| \frac{k_i - k_1}{k_2 - k_1} \right|.
\]

A stability domain of the scheme (15) is shown on a Fig. 1.

\[
\text{Fig. 1 Stability domain of the scheme (15)}
\]

A stability interval of (15) of second accuracy order is approximately equal to two. Therefore, an inequality \( w_{n,2} \leq 2 \) can be applied for stability control. In case of using this inequality for step selection, roughness of estimation (16) should be considered, because a maximum eigenvalue may not be strongly separated from rest, in a power method few iterations are applied and additional distortions occur, because of nonlinearity of the problem (1). Therefore, stability control is used to limit size of an integration step. As a result, we will calculate the projected step \( h_{n+1} \) as follows. We define a new step \( h^\omega \) by criterion of accuracy according to the formula
\[
h^\omega = dh_n, \quad d, \quad \text{taking into account a relation} \quad k_2 - k_1 = O(h^\omega),
\]

is given by an equation
\[
q^2 \|k_2 - k_1\| = \varepsilon.
\]

A step \( h^\omega \) by criterion of stability is given by a formula
\[
h^\omega = dh_n, \quad \text{where} \quad d, \quad \text{taking into account a relation} \quad w_{n,2} = O(h). \quad \text{is determined from an equation} \quad dw_{n,2} = 2. \quad \text{Then,} \quad \text{the projected step} \quad h_{n+1} \quad \text{is calculated by a formula}
\]
\[
h_{n+1} = \max \left[ h_n, \min \left( h^\omega, h^\omega \right) \right].
\]

Note, that the formula (17) is used to predict size of the integration step \( h_{n+1} \), after successful computation of solution with the previous step \( h_n \) and, therefore, does not actually lead to increase of computational cost. If the step by criterion of stability is less than the last successful one, it will not be reduced, because it may be caused by roughness of estimation of a maximum eigenvalue. However, the step will not be increased, because there is a possibility of instability of the numerical scheme. If the step should be reduced by criterion of stability, then the latest successful step \( h_n \) is applied again. As a result, the formula (17) is proposed to select a step. This formula allows to stabilize step behavior on a settling region of solution, where stability has a defining role. Indeed, existence of this region limits possibilities of applying explicit methods for solving stiff problems.

IV. FIRST ORDER RUNGE-KUTTA METHOD

For numerical solution of the problem (1), we consider a scheme
\[
y_{n+1} = y_n + \tau k_1 + \tau k_2, \quad (18)
\]

\[
k_1 = hf(y_n), \quad k_2 = hf(y_n + k_1).
\]

Note, that when \( \tau = r_1 = 0.5 \), the numerical formula (18) has second order of accuracy, and coincides with (15) with coefficients \( p_1 = p_2 = 0.5 \). We construct a less accurate scheme with a maximum interval of stability. For this purpose, we use (18) for solution the scalar test equation (7). We obtain
\[
y_{n+1} = Q(x)y_n, \quad \text{where the function of stability} \quad Q(x) \quad \text{has a form}
\]
\[
Q(x) = 1 + (r_1 + r_2)x + r_2 x^2, \quad x = h\lambda.
\]

Requirement of first order of accuracy leads to the relation
\[
r_1 + r_2 = 1,
\]

which, below, we will assume to be satisfied. Now, we choose \( r_2 \), so that the method (18) has a maximum stability interval. For this purpose, we consider the Chebyshev polynomial
\[ T_2(z) = (2z^2 - 1) \]
on an interval [-1,1]. We carry out change of variables, setting
\[ z = 1 - \frac{2}{\gamma} x. \]
We obtain
\[ T_2(x) = 1 - \frac{8}{\gamma} x + \frac{8}{\gamma^2} x^2, \]
and the interval \([\gamma, 0]\) passes to [-1,1]. It is easy to show, that among all polynomials of a form
\[ P_2(x) = 1 + x + c_2 x^2 \]
for \( T_2(x) \) the inequality \(|T_2(x)| \leq 1\) is satisfied at a maximum interval \([\gamma, 0]\), \( \gamma = -8 \). We require, that the coefficients of \( Q(x) \) and \( T_2(x) \) coincide at \( \gamma = -8 \). This leads to relations
\[ r_1 + r_2 = 1, \quad r_2 = \frac{1}{8}. \]
As a result, we have coefficients
\[ r_1 = \frac{7}{8}, \quad r_2 = \frac{1}{8} \]
of the first accuracy order method with a maximum stability interval, with a local error
\[ \delta_h = \frac{3}{8} h^2 f' f + O(h^3). \]
We will use estimation of the local error to control accuracy of the numerical formulas of the first order. Taking into account, that
\[ k_2 - k_1 = h^2 f'_h f_h + O(h^3) \]
and a form of the local error, an inequality for accuracy control can be written as
\[ \|k_2 - k_1\| \leq \frac{8}{3} \epsilon, \]
where \( \| \cdot \| \) is some norm in \( R^N \), \( \epsilon \) is required accuracy of calculations.
We construct an inequality for stability control for a first order method. For this purpose, we consider an auxiliary stage
\[ k_1 = hf(y_{n+1}). \]
We write \( k_1, k_2, \) and \( k_1, \) applied to the problem \( y' = Ay \), where \( A \) is the matrix with constant coefficients. As a result, we obtain
\[ k_1 = Xy_n, \quad k_2 = (X + X^2)y_n, \]
\[ k_3 = \left( X + X^2 + \frac{1}{8} X^3 \right)y_n, \]
where \( X = hA \). It is easy to see, that
\[ k_2 - k_1 = X^2 y_n, \quad 8(k_2 - k_3) = X^3 y_n. \]
Then, according to [9], estimation of a maximum eigenvalue \( w_{n,1} = h \lambda_{n,\text{max}} \) of the Jacobi matrix of the system (1) can be calculated by a formula
\[ w_{n,1} = 8 \max_{\text{over } \lambda} \left\{ \frac{|k_1 - k_2|}{|k_2 - k_1|} \right\}. \]
A stability domain of the scheme (18) is shown on a Fig. 2.

An interval of stability of the numerical scheme (18) is equal to eight. Therefore, an inequality \( w_{n,1} \leq 8 \) can be applied to control stability.

V. ALGORITHM WITH AUTOMATIC SELECTION OF A NUMERICAL SCHEME

An algorithm of alternating order and step can be easily formulated on a base of constructed explicit methods of first and second orders of accuracy. Calculations are always begun with the second order method as it is more accurate. Transition to the first order scheme is carried out in case of violation an inequality \( w_{n,2} \leq 2 \). Reverse transition to the second order method is carried out if an inequality \( w_{n,1} \leq 2 \) holds. On calculations by the first order method in addition to accuracy control there is stability control, and choice of a projected step is carried out in the same manner as in the second order method applying a formula of type (17).

Using the scheme (2) does not present difficulties. Violation of an inequality \( w_{n,1} \leq 8 \) causes a transition to the scheme (2). Transfer to explicit methods is carried out if an inequality \( w_{n,2} \leq 8 \) holds.

The numerical formula (2), without the loss of the accuracy order, can be applied with the frozen matrix \( D_n \). Note, that during the freezing the Jacobi matrix, size of an integration step remains constant. An attempt to freeze the matrix \( D_n \) is carried out after each successful step. The matrix thaws in the following cases: (1) violation of accuracy of calculations; (2) if number of steps with a frozen matrix reaches a defined maximum number \( i_h \); (3) if a projected step is greater than the last one by \( q_h \) times. By the numbers \( i_h \) and \( q_h \) we can affect the redistribution of computational cost. When \( i_h = 0 \) and \( q_h = 0 \), freezing does not occur; with increasing \( i_h \) and \( q_h \), the number of calculations of a right part increases, while the number of inversions of the Jacobi matrix decreases.

The norm in a left part of inequality for accuracy control is calculated by a formula
\[ \|k_2 - k_1\| = \max_{i \in \mathbb{N}} \left\{ \frac{|k'_i - k'_i|}{|y'_i| + r} \right\}, \]

where \(i\) is a number of component, \(r\) is a positive parameter.

If, for the \(i\)-th component of solution, an inequality \(|y'_i| < r\) holds, then an absolute error \(re\) is controlled, otherwise, the relative error \(\varepsilon\) is controlled. Below, the algorithm of alternating order and step with automatic selection of an explicit or a \(L\)-stable numerical scheme is called RKMK2.

### VI. DIFFERENTIAL EQUATIONS OF CHEMICAL KINETICS

The kinetic scheme of any chemical reaction includes the following elementary reactions (stages)

\[ a_1 x_1 + \ldots + a_{NR} x_{NR} \rightarrow \beta_1 x_1 + \ldots + \beta_{NR} x_{NR} \]

\[ \ldots \ldots \]

\[ a_1 x_1 + \ldots + a_{NR} x_{NR} \rightarrow \beta_1 x_1 + \ldots + \beta_{NR} x_{NR} \]

where \(x_i\), \(1 \leq i \leq NR\) are chemical reagents, \(NR\) and \(NS\) are numbers of the reagents and the stages in the reaction, respectively; \(a_j\) and \(\beta_j\), \(1 \leq i \leq NR\), \(1 \leq j \leq NS\) are the stoichiometric coefficients. For each elementary reaction a corresponding stage velocity constant \(k_j\), \(1 \leq j \leq NS\) is given.

For process (19) under the lumped model of an isothermal reactor of constant capacity the corresponding ordinary differential equations system has the following form

\[ C' = A^T V, \quad C(0) = C_0. \]

Here, \(A^T\) is a stoichiometric matrix, \(C\) and \(V\) are vectors of reagents concentrations and stage velocities, respectively. When a reaction proceeds in non-isothermal conditions, this system also involves the heat balance equation

\[ T' = \frac{\frac{Q'}{C^T} - \alpha(T - T_{in})}{C^T C} - \frac{1}{\Theta}(T - T_{in}), \]

where \(T\) is mixture temperature in a reactor, \(T_{in}\) is temperature of walls of a reactor, \(\frac{Q'}{C^T}\) is the vector of calorific capacities of the stages, \(\alpha\) is a vector of heat capacities of the reagents, \(\alpha = \tilde{as}\), \(s\) and \(r\) are square of an area and volume of the reactor, respectively. The superscript \(T\) of the vectors \(\frac{Q'}{C^T}\) and \(C^T\) denotes the transposition. The heat capacities of the reagents and the heat-conduction coefficient may be functions of the reagents concentrations \(c_i\), \(1 \leq i \leq NR\), \(\alpha\) may depend on temperature.

If a reaction proceeds in an isothermal reactor of constant capacity with substance exchange (an open system, a perfect-mixing reactor), a system of ordinary differential equations has a form

\[ C' = A^T V + \frac{1}{\Theta}(C_p - C), \quad C(0) = C_0, \]

where \(C_p\) is a vector of inlet reagent concentrations, \(\Theta = r/u\) is a stay period of mixture in a reactor, \(u\) is mixture space velocity. If a reaction proceeds in non-isothermal conditions, then this system also involves a heat balance equation

\[ T' = \frac{\frac{Q'}{C^T} - \alpha(T - T_{in})}{C^T C} - \frac{1}{\Theta}(T - T_{in}), \]

where \(T_{in}\) is inlet mixture temperature in a reactor. The temperature of reaction mixture can be described by a function of time \(t\) and concentrations of reagents \(c_i\), \(1 \leq i \leq NR\), i.e.

\[ T = T(t, C). \]

### VII. ALGORITHM FOR GENERATING CHEMICAL KINETIC EQUATIONS

If an elementary reaction is balancing, its velocity \(W_s\) is equal to a difference of its forward \(W_s^+\) and backward \(W_s^-\) reactions, i.e. \(W_s = W_s^+ - W_s^-\), \(1 \leq s \leq NS\). If there is some third entity in a reaction, the velocity \(V_s\) is calculated by formulas

\[ V_s = P W_s, \quad P = \sum_{i=1}^{NR+NI} e_{ij} c_i, \quad 1 \leq s \leq NS, \]

where \(e_{ij}\), \(1 \leq s \leq NS\), \(NR+1 \leq i \leq NR+NI\), are efficiencies of the third entities, \(NI\) is number of inert substances, \(c_i\) and \(c_s\) are efficiencies and concentrations of the inert substances, respectively. Values of components of the vector \(W_s\) are determined from a scheme of a chemical reaction (19) by relations

\[ W_s^+ = k_j \prod_{i=1}^{NR+NI} e_{ij}^{c_i}, \quad W_s^- = k_{-j} \prod_{i=1}^{NR+NI} e_{ij}^{c_i}, \]

where \(k_j\) and \(k_{-j}\), \(1 \leq s \leq NS\), are forward and backward velocity stage constants, respectively. Velocity constants of the stages are calculated using the formulas

\[ k_j = A_j T^{n_j} \exp \left( \frac{-E_j}{RT} \right), \]

where \(T\) is temperature of mixture in a reactor; \(A_j\), \(n_j\) and \(E_j / R\) are given constants. Note, that, in general, the velocity constants values are not constant in case of a non-isothermal reactor – they depend on temperatures. However, historically, an isothermal reactor was considered earlier than non-isothermal one and thus \(k_j\), \(1 \leq j \leq NS\), at the present time, are still called constants. The stoichiometric matrix \(A^T\) with elements \(a_{ij}\) is formed from the kinetic scheme (19) conforming to the following rule. A number of a stage is aligned with a column number and a reagent number is aligned with a row number of a matrix \(A^T\). If \(x_i\) is an initial reagent, then \(a_{ij} = -a_{ij}\), if \(x_i\) is a product, then \(a_{ij} = \beta_{ij}\). Usually, a few amount of reagents are reacting in a stage, i.e. a stoichiometric matrix is sparse.
VIII. NUMERICAL RESULTS

Calculations were carried out on PC Intel(R) Core(TM) i7-3770S CPU@3.10GHz with double precision. In the calculations, the parameter \( r \) was chosen so that practical accuracy of all components of solution was not worse than required accuracy. Calculations were performed with defined accuracy \( \varepsilon = 10^{-2} \). This is due to the fact, that the algorithm is based on low accuracy order schemes, and, therefore, it is impractical to carry out calculations with higher accuracy with this method. A comparison of its efficiency was carried out with the well-known Gear method in the implementation of A. Hindmarsh named DLSODE from the ODEPACK collection \[5\].

Below \( i_y \) and \( i_y \) denote, respectively, total numbers of calculations of a right part and number of inversions (decompositions) of the Jacobi matrix of the problem (1), which allow us to evaluate objectively the efficiency of the integration algorithm.

As the first test, the simplest model of the Belousov-Zhabotinsky reaction \[14\] was chosen

\[
y_i' = \begin{cases} 7.727 (y_2 - y_1 y_2 + y_1 - 8.375\cdot 10^{-\varepsilon} y_1^2), \\ 1 \end{cases} \quad (20)
\]

\[
y_i = 0.161 (y_1 - y_3), \quad y_i(0) = y_i(0), \quad t \in [0, 300], \quad h_y = 2 \cdot 10^{-3}.
\]

Calculations were carried out with the numerical Jacobi matrix.

A solution of this problem by the algorithm RKM2 was calculated with costs \( i_y = 1214 \) and \( i_y = 65 \). Calculations only by the \( L \)-stable scheme (2) give \( i_y = 926 \) and \( i_y = 88 \). Practical accuracy of the calculations at the end of the interval of integration is not worse than required one. Solution of (20) was calculated by explicit methods of alternating order and step with cost \( i_y = 2 \cdot 116278 \). This problem is too stiff for shown here to demonstrate principal possibility of application explicit methods for solving stiff enough examples, those in solving some high-dimensional problems may be more efficient than \( L \)-stable methods. For calculations by the DLSODE program, the required accuracy \( 10^{-2} \) is achieved, when the defined accuracy equal is \( 10^{-4} \) with costs \( i_y = 1129 \) and \( i_y = 107 \). On calculations with higher accuracy, DLSODE is more efficient than the constructed algorithm. This is a sequence of low accuracy order of the constructed numerical formulas. On defined accuracy equal to \( 10^{-2} \), the algorithm RKM2 is more efficient than the well-known method DLSODE in 1.5 times in number of inversions of the Jacobi matrix, while number of computations of the right part of (20) for RKM2 and DLSODE vary slightly. In case of the large-scale problem (1), the constructed integration algorithm may be more efficient than DLSODE in calculating time. The time dependence of \( y_1 \) is showed on a Fig. 3.

A second example describes the modified oregonator exhibiting complicated limit cycle. This reaction includes following six elementary stages \[15\]

\[
A + Y \rightarrow X + P, \quad k_1 = 0.084, \quad k_2 = 1.0^4,
\]

\[
X + Y \rightarrow 2P, \quad k_2 = 4 \cdot 10^8, \quad k_3 = 5 \cdot 10^5,
\]

\[
A + X \rightarrow 2W, \quad k_3 = 2 \cdot 10^7, \quad k_3 = 2 \cdot 10^7,
\]

\[
C + W \rightarrow X + Z, \quad k_4 = 1.3 \cdot 10^7, \quad k_4 = 2.4 \cdot 10^7,
\]

\[
2X \rightarrow A + P, \quad k_5 = 4 \cdot 10^7, \quad k_5 = 4 \cdot 10^{-11},
\]

\[
Z \rightarrow C + 0.462 Y, \quad k_6 = 0.65,
\]

where \( k_i \), \( 1 \leq i \leq 6 \), velocity constants of forward (with positive indices) and backward (with negative indices) elementary stages. There are 7 entities in this reaction, denoted by

\[
A = BrO_3, \quad C = M(n), \quad P = HOBr,
\]

\[
W = BrO_2, \quad X = HBrO_2, \quad Y = Br^-, \quad Z = M(n+1).
\]

In these notations \( M(n) \) is an ion of metal accelerant, \( M(n+1) \) is an oxygenated form of the ion. Let's denote concentrations of reagents by

\[
c_1 = [BrO_3], \quad c_2 = [Br^-], \quad c_3 = [M(n)],
\]

\[
c_4 = [HBrO_2], \quad c_5 = [HOBr], \quad c_6 = [BrO_2], \quad c_7 = [M(n+1)].
\]

This reaction proceeds in an isothermal reactor with constant capacity with substance exchange. A corresponding system of equations is given below

\[
c_1' = -v_1 - v_3 + v_5 + \frac{1}{\Theta} (c_{p1} - c_1),
\]

\[
c_2' = -v_1 - v_2 + 0.462 v_6 + \frac{1}{\Theta} (c_{p2} - c_2),
\]

\[
c_3' = -v_4 + v_6 + \frac{1}{\Theta} (c_{p3} - c_3),
\]

\[
c_4' = v_1 - v_2 - v_3 + v_4 - 2 v_5 + \frac{1}{\Theta} (c_{p4} - c_4),
\]

\[
c_5' = v_1 + 2 v_2 + v_3 + \frac{1}{\Theta} (c_{p5} - c_5),
\]

\[
c_6' = 2 v_3 - v_4 + \frac{1}{\Theta} (c_{p5} - c_5),
\]

\[
c_7' = v_4 - v_6 + \frac{1}{\Theta} (c_{p7} - c_7).
\]
where $\Theta = 125.5$ and velocities $v_1$, $v_2$, ..., $v_6$ of stages are defined by formulas:

$v_1 = k_1 c_1^2 - k_3 c_3 c_5$, $v_2 = k_2 c_2^2 - k_3 c_3^2$, $v_3 = k_4 c_4^2 - k_3 c_3 c_7$, $v_4 = k_6 c_6^2 - k_3 c_3 c_7$, $v_5 = k_5 c_4^2 - k_3 c_3 c_7$, $v_6 = k_7 c_7$.  

Integration of the system (21) was made on an interval $[0,1000]$ with an initial step equal to $10^{-5}$. Inlet concentrations of reagent are given below,

$c_{p1} = 0.14$, $c_{p2} = 0.151 \cdot 10^{-5}$, $c_{p3} = 0.125 \cdot 10^{-3}$, $c_{p4} = c_{p5} = c_{p6} = c_{p7} = 0$.

Initial values of reagent concentrations are equal to

$c_1 = 0.1387$, $c_2 = 0.1534 \cdot 10^{-6}$, $c_3 = 0.1176 \cdot 10^{-3}$, $c_4 = 0.3165 \cdot 10^{-7}$, $c_5 = 0.1956 \cdot 10^{-3}$, $c_6 = 0.5814 \cdot 10^{-6}$, $c_7 = 0.631 \cdot 10^{-5}$.

Time dependence of $[\text{BrO}_2]$ is showed on a Fig. 4.

Calculations were performed with the numerical Jacobi matrix. Solution of the problem was calculated by the algorithm RKMK2 with $i_f = 5,623$ and $i_j = 533$. Calculations with the $L$-stable scheme (2) only give $i_f = 5,371$ and $i_j = 591$. Practical accuracy in the end of the integration interval is as good as defined one. In calculations by DLSODE required accuracy $10^{-2}$ is achieved for defined accuracy equal to $10^{-4}$ with computational costs $i_f = 7,806$ and $i_j = 542$. On higher accuracy of calculations DLSODE is more efficient than the constructed algorithm. It is a result of low order of accuracy of constructed numerical formulas. In case of high dimension of the problem (1) the constructed algorithm may be more efficient in time than DLSODE.

IX. CONCLUSION

The constructed algorithm RKMK2 is designed for low precision calculations — about 1% and lower. In this case, its maximum efficiency is reached.

In RKMK2, with its parameters, one can specify different modes of calculations:

(1) explicit methods of first or second order of accuracy with or without stability control;
(2) explicit methods of alternating order and step;
(3) $L$-stable method with or without freezing, both an analytical and a numerical Jacobi matrix.
(4) with automatic selection of a numerical scheme.

This allows us to apply this algorithm to solving both stiff and non-stiff problems. In calculations with automatic selection of a numerical scheme, the integration algorithm makes a decision whether a problem is stiff or not by itself.

Using the inequality for stability control does not actually lead to increase of computational cost, because estimation of a maximum eigenvalue of the Jacobi matrix of (1) is carried out through a previously computed stages and does not lead to increase of number of computed values of function $f$. This estimation is rough. However, using stability control for limiting the step growth allows us to avoid the negative effects of roughness of estimation. Moreover, in some cases this leads to an exceptionally high growth of efficiency of the algorithm.

In a settling region, the old errors tend to zero due to stability control and new ones are low, due to small values of derivatives of a solution. In some cases, following eigenvalue is estimated instead of a maximum one. An integration step becomes greater than a maximal admissible one, and with such a step the integration is carried out as long as the inequality for accuracy control is not violated. Typically, the number of such steps is small. However, the step may be an order of magnitude greater than the maximum step by a criterion of stability. After violation of the inequality for accuracy control, the step is reduced to a maximum admissible. This effect may occur many times, depending on length of a region of settling. As a result, an average integration step may be greater than the maximum admissible one.

Application of the explicit first order method with an extended stability domain on a settling region allows us to increase step size by 4 times in comparison with the explicit second order method without increasing of computational cost. On transition regions, where accuracy of calculations has a defining role, the second accuracy order method is more efficient, though it has rather small stability domain.

Combining methods of low and high orders applying an inequality for stability control, improves efficiency of calculations.

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