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ALTERNATING ORDER ALGORITHM BASED ON STAGES OF CESCHINO'S METHOD

ABSTRACT. This paper investigates the methods for numerical solution of stiff problems with large dimension. Using the estimation of the largest eigenvalue of the Jacobi matrix it has been constructed an inequality in order to control the stability of a Cescino numerical scheme with second-order accuracy. To integrate a variable step it is proposed a formula which allows predicting the next step in time. On the basis of this formula, it has been developed a method with first-order accuracy with extended stability range. This method allows stabilize behavior of step integration at the stage of solution exactly where stability plays a crucial role. This makes it possible to remove restrictions on the possibility of using explicit methods for solving stiff problems. It has been formulated an algorithm for the numerical solution of stiff problems of variable order, which uses the irregular step in time with an additional control of stability of the numerical integration scheme. This paper demonstrates solutions of stiff problems associated with numerical simulations of ethane pyrolysis, which confirm an increase in efficiency due to the use of variable order.

KEY WORDS. Explicit methods, control accuracy and stability, stiff problems.

Introduction. For numerical solution of large dimensional stiff problems it is necessary to use algorithms based on explicit methods [1–3]. The methods of integration based on implicit or semi-explicit numerical schemes usually use the Jacobi matrix inversion [2]. In this case it is a separate time-consuming problem. In such a situation it is preferable to use algorithms based on explicit formulas, if the stiffness of the problem allows to get the approximation to the solution within a reasonable time [3].

The control algorithm of the integration step is usually based on the control accuracy of the numerical scheme. This is natural, because the main criterion is the accuracy of finding a solution. However, with the usage of integration algorithms based on explicit formulas to solve stiff problems, this approach leads to a loss of efficiency and reliability [4–5]. This is due to the fact that on the setting area the contradiction between accuracy and resistance leads to a large number of repeated calculations solutions, and the step is selected significantly lower than the permissible maximum. This can be prevented by additional stability control of the numerical scheme. At present there are two approaches to the control of stability [5–7]. The first one is connected with the assessment of the maximum eigenvalue of the Jacobi matrix

through its norm with the subsequent control (along with accuracy) of inequality $h\|f_y'\| \le D$ [6], where D is a positive constant related to the size of the stability domain. It is clear that for explicit methods where the Jacobi matrix is not involved in the computation process, this additionally results in its finding and consequently to the increase of computational expenditures. The second approach is based on the estimation of the largest eigenvalue of the Jacobi matrix λ_{max} with the power method through the right side increments of the system of differential equations with the subsequent control of the inequality $h|\lambda_{max}| \le D$ [7]. In all these cases this assessment does not increase the calculation consumptions [3–5, 7]. Here, using the proposed in [7] the estimation method of the largest eigenvalue of the Jacobi matrix we establish an inequality in order to control the stability of a Cescino numerical scheme with second-order accuracy [8]. Numerical results confirm the efficiency of the integrating algorithm due to the stability control.

Cescino method. Cauchy problem is under consideration

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

where y and f—N-dimensional material vector functions, t—independent variable that varies on a given interval $[t_0, t_k]$. To solve the task (1) we use explicit formulas of Runge-Kutta

$$\begin{aligned} &y_{n+1} = y_n + p_{m1}k_1 + p_{m2}k_1 + p_{m3}k_3 + p_{m4}k_4,\\ &k_1 = hf(t_n, y_n),\ k_2 = hf(t_n + h/4, y_n + k_1/4),\\ &k_3 = hf(t_n + h/2, y_n + k_2/2),\ k_4 = hf(t_n + h, y_n + k_1 - 2k_1 + 2k_1), \end{aligned} \tag{2}$$

where h—the integration step, k_i, $1 \le i \le 4$ — stages of the method, p_{mi}, $1 \le i \le 4$ — numerical coefficients, m—order of the method accuracy. When the coefficients are

$$p_{21} = 1,\ p_{22} = 2,\ p_{23} = 2,\ p_{24} = 0, \tag{3}$$

the scheme (2), (3) has the second-order accuracy [8].

Control of calculation accuracy. Scheme (2) with coefficients

$$p_{41} = 1/6,\ p_{42} = 0, p_{43} = 2/3,\ p_{44} = 1/6$$

has the fourth order. Then for accuracy control of the second order scheme error estimate can be used $\delta_{n,2}$ of type

$$\delta_{n,2} = (p_{41} - p_{21})k_1 + (p_{42} - p_{22})k_2 + (p_{43} - p_{23})k_3 + (p_{44} - p_{24})k_4.$$

As a result for the control of the calculation accuracy we use the inequality $\|\delta_{n,2}\| \le \varepsilon$, where $\|\cdot\|$—some norm in R^N, ε—the required calculation accuracy.

Taking into consideration we have the relation $\delta_{n,2} = O(h^3)$, step h^{ac} for accuracy is chosen according to the formula $h^{ac} = qh$, where q index is calculated by the equation $q^3\|\delta_{n,2}\| = \varepsilon$. If $q < 1$ the solution (return) re-evaluation is done with step h, equal to qh. Otherwise, the approximate solution is computed and the predicted step h_{n+1} is calculated according to the formula $h_{n+1} = qh$.

Inequality $\|\delta_{n,2}\| \le \varepsilon$ has proved itself for solving many practical problems, and it will be used below. The following variable step algorithm based on schemes (2), (3) with the inequality for accuracy control $\|\delta_{n,2}\| \le \varepsilon$ is CESCH42.

Control of numerical scheme stability. Let us construct the inequality to control the stability of the scheme (2). To do this we apply (2) to solve the linear equation $y' = Ay$ with a constant matrix A. The first three stages k_1, k_2 и k_3 in relation to this problem have the form

$$k_1 = Xy_n,\ k_2 = (X + X^2/4)y_n,\ k_3 = (X + X^2/2 + X^3/8)y_n$$

where $X = hA$. It is easy to see that we have the relations

$$k_1 - 2k_2 + k_3 = X^3 y_n/8,\ 0.5(k_2 - k_1) = X^2 y_n/8.$$

Now we can calculate the estimation of the largest eigenvalue of the Jacobi matrix of the system (1) with the help of the power method [3]. We introduce the notation

$$v_n = 2 \cdot \max_{1 \le i \le N} \{|(k_1 - 2k_2 + k_3)_i| / |(|(k_2 - k_1)_i|)|\}. \qquad (4)$$

Then to control the stability of the Cescino method we can use the inequality $v_n \le D$, where number D limits the stability interval.

The stability of methods of Runge-Kutta type is usually studied on the scalar test equation $y' = \lambda y$, where λ is an arbitrary complex number, $\mathrm{Re}(\lambda) < 0$.

The meaning of λ—some eigenvalue of the Jacobi matrix task (1).

Applying (2), (3) to solve $y' = \lambda y$ we find out that the stability function $Q_2(x)$ of second order accuracy method is the following

$$\mathrm{Q_2(x) = (1 + X + X\ 2/2 + X\ 3/4),\ x = h\lambda}$$

and the stability function $Q_4(x)$ of the fourth-order method is as follows

$$Q_4(x) = (1 + X + X^2/2 + X^3/6 + X^4/24),\ x = h\lambda.$$

The stability interval of the second-order method is two, and the fourth-order scheme is approximately 2.8. Therefore we set $D = 2$ in the inequality $v_n \le D$. Considering that $v_n = O(h)$, a step for h^{st} to the stability can be chosen by the formula $h^{st} = rh$, where r is computed from the equation $rv_n = 2$.

Rating (4) is rough, because it is not necessarily that the largest eigenvalue is strongly separated from the other eigenvalues. In a power method little iteration is used and nonlinearity problem (1) introduces additional distortions. Therefore, the stability control is used as a constraint on the size of the integration step. As a result, the predicted step is calculated by the formula

$$h_{n+1} = \max\{h_n, \min[h^{ac}, h^{st}]\} \qquad (5)$$

where h_n is the last successful integration step. We note that the formula (5) is used to forecast the magnitude of the integration step h_{n+1} after a successful computing solutions with the previous step h_n, and so in fact it does not increase the computational expenditures. If the step on the stability is less than the last successful it will not be reduced because the reason for this may be the roughness of the largest eigenvalue

estimation. However, the step will not be increased because the possibility of the numerical scheme instability is not excluded. If the step on the stability should be reduced, then the next step will be the last successful step h_n. As a result, we use the formula (5) to choose a step.

This formula allows us to stabilize the behavior of the step on the establishment decision section where stability plays a decisive role. The presence of this section severely limits the use of explicit methods for solving stiff problems.

Later the variable step algorithm with additional control stability of the numerical scheme we will call CESCH42st. This algorithm is based on a numerical formula of low (second) order accuracy, and therefore it is aimed at solving non-rigid problems with low precision calculations (about 1% or less), as well as problems of moderate stringency. From the results of calculations algorithm CESCH42st follows that the actual accuracy of the calculations in the setting area is much higher than the given one. This is natural, because in this sector the old errors are suppressed due to the stability control, and new errors are small due to the smallness of the solution derivatives. In such a situation it is more effective to carry out calculations on the low-order method with a wider stability.

First-order method. Based on stages of the numerical scheme (2) we construct a method of the first-order accuracy of type

$$y_{n+1,1} = y_n + p_{11}k_1 + p_{12}k_1 + p_{13}k_3 + p_{14}k_4 \qquad (6)$$

with a wider area of stability. For this we use (6) to solve the test equation $y' = \lambda y$.

We get $y_{n+1} = Q_1(x)y_n$ where $x = h\lambda$, stability function $Q_1(x)$ has the form

$$Q_1(x) = 1+(p_{11}+p_{12}+p_{13}+p_{14})x+(p_{12}/4+p_{13}/2+p_{14})x^2+(p_{13}/8+p_{14}/2)x^3+p_{14}x^4/4. \qquad (7)$$

The requirement for a first-order accuracy numerical formula (7) implies the implementation of correlation $p_{11} + p_{12} + p_{13} + p_{14} = 1$. The remaining coefficients p_{1i} are used to extend the stability area. Stability condition of the scheme (6) has the form $|Q_1(x)| \le 1$. To construct a method with a maximum stability interval we consider the Chebyshev polynomial of the form $T_4(z) = 8z^4 - 8z^2 + 1$. It is known that the polynomial $T_4(z)$ has the least deviation from zero at $z \in [-1,1]$. We make the change of variables $z = 1 - 2x/\gamma$, while the segment $[\gamma,0]$ is displayed on the interval $[-1,1]$. As a result, polynomial $T_4(x)$ can be written as

$$T_4(x) = 1 - 32x/\gamma + 160x^2/\gamma^2 - 256x^3/\gamma^3 + 128x^4/\gamma^4. \qquad (8)$$

It is easy to show [3] that the inequality $|T_4(x)| \le 1$ for $T_4(x)$ is executed at the maximum interval $[\gamma,0]$, $\gamma = 32$. Comparing the correlations (7) and (8) with $\gamma = 32$, we get the coefficients p_{1i}, $1 \le I \le 4$, of the first order accuracy method (2) with a maximum interval of stability, that is

$$p_{11} = 895/2048, p_{12} = 257/512, p_{13} = 31/512, p_{14} = 1/2048. \qquad (9)$$

The stability area of the first-order method (6), (9) along the real axis is 16 times wider than the stability area of the numerical scheme (2), (3). Computational

expenditures the first-order method and the second-order are the same. Therefore, for tasks in which the step is limited mainly by the stability, the offered theoretical efficiency is of 16 times.

Accuracy and stability control of the method (6) and (9). In the inequality for accuracy control we will apply the local error estimation.

$$\delta_{n,1} = (p_{41} - p_{11})k_1 + (p_{42} - p_{12})k_2 + (p_{43} - p_{13})k_3 + (p_{44} - p_{14})k_4.$$

Then to control the accuracy of the numerical formula (6) and (9) we can apply the inequality $|\delta_{n,1}| \le \varepsilon$. Further, since the stability interval of the numerical scheme (6), (9) is limited by the number 32, then for its stability control we can use the inequality $v_n \le 32$, where v_n is found by the formula (4).

Algorithm of variable order. First-order methods with extended stability ranges are effective in the establishing areas where the step is limited by stability.

At high precision of calculations at transition points method (2), (3) will be more effective. The increase in efficiency can be achieved by the use of each method on the area where it is most effective. As a criterion for switching from one method to another the inequality can be used to control the stability. In the calculations by the method (2), (3) the transition to the numerical scheme (6), (9) is carried out in violation of inequality $v_n \le 2$. In the calculations by the first-order method the reverse transition occurs in the case when $v_n \le 2$. Calculations by the first order method are accompanied by additional (along with accuracy) control of inequality $v_n \le 32$, and the step is chosen according to the formula of the type (5).

Differential equations of chemical kinetics. The kinetic scheme of the chemical reaction consists of elementary stages of the form

$$\alpha_{1,1}x_1 + \ldots + \alpha_{NR,1}x_{NR} \to \beta_{1,1}x_1 + \ldots + \beta_{NR,1}x_{NR}, \qquad (10)$$

$$\alpha_{1,NS}x_1 + \ldots + \alpha_{NR,NS}x_{NR} \to \beta_{1,NS}x_1 + \ldots + \beta_{NR,NS}x_{NR}$$

where x_i, $1 \le i \le$ NR—reagents; NR и NS—correspondingly the number of reagents and the number of stages in the reaction; α_{ij} and β_{ij}, $1 \le i \le$ NR, $1 \le j \le$ NS — stoichiometric coefficients. For each elementary reaction the rate constants of stages are given k_j, $1 \le j \le$ NS. A system of ordinary differential equations $C' = A^T V$c with given initial condition $C(0) = C_0$ corresponds to the process (10) within the lumped model of constant volume isothermal reactor. Here A^T—stoichiometric matrix, C и V—respectively, the vector of reactant concentrations and rates of stages. In the case of the reaction in the non-isothermal conditions the system heat balance equation $T' = \{Q^T V - \alpha(T - T_{01})\}/\{C_V{}^T C\}$ is added where T—temperature of the mixture in the reactor, T_{01}—temperature of the reactor walls, Q^T—vector of unit heats stages, $C_V{}^T$—heat capacities reactant vector, $\alpha = \acute{\alpha}s/r$, $\acute{\alpha}$—heat transfer coefficient, s and r—surface area and reactor volume. The upper index T of the vectors Q^T and $C_V{}^T$ stands for transposition. The heat capacities of reagents and heat transfer coefficient can be functions of the reagent concentrations c_i, $1 \le i \le$ NR, and α may also depend on the temperature.

If the reaction occurs in an isothermal reactor of constant volume with substance exchanges (open system, ideal mixing reactor), the system of differential equations can be written as $C' = A^T V + (C_p - C)/\Theta$, where C_p—vector reagents concentration at the reactor inlet, Θ—residence time of the mixture in the reactor, $\Theta = r/u$, u—volumetric flow rate of the mixture through the reactor. When the reaction takes place in non-isothermal conditions, the system is supplemented by the heat balance equation $T' = \{Q^T V - \alpha(T - T_{01})\}/(C_V{}^T C) - (T - T_{02})/\Theta$ where T_{02}—the temperature of the mixture at the reactor inlet. The temperature of the reaction mixture may be given as a function of time t and reagents concentration c_i, $1 \le I \le N_r$, that is $T = T(t,C)$.

Algorithm of formation of chemical kinetics equations [9]. If the stage is reversible, the speed stage W_s is the difference in velocity of direct W^+_s and inverse W^-_s processes, that is $W_s = W^+_s - W^-_s$, $1 \le s \le$ NS. If the third particle is involved in the stage, the speed V_s is calculated by the formulas

$V_s = P_s W_s$, $P_s = \sum_{i=1}^{NR+NI} \varepsilon_{si} c_i$, $1 \le s \le$ NS

where ε_{si}, $1 \le s \le$ NS—effectiveness of third particles, NI—the number of inert substances, ε_{si} и c_i, NR + 1 $\le I \le$ NR + NI—efficiency and concentration of inert substances. The values of the vector W_so components are determined from the chemical reaction scheme (10) according to relations

$$W^+_s = k_s \prod_{i=1}^{NR+NI} c^{\alpha ij}, \; W^-_s = k_{-s} \prod_{i=1}^{NR+NI} c^{\beta ij}$$

where k_s and k_{-s}, $1 \le s \le$ NS—the rate constants of direct and inverse stages, respectively. Rate constants of stages are calculated by the formulas

$$k_j = A_j T^{nj} \exp(-E_j/[RT])$$

where T—temperature of the mixture in the reactor; A_j, n_j и E_j/R—given constants.

It is important to note that, in general, the rate constants in the case of non-isothermal reactor are not permanent—they depend on the temperature. However, at first historically an isothermal reactor was considered and k_j, $1 \le i \le$ NS are still called constants now.

The stoichiometric matrix A^T with elements a_{ij} is formed out of the kinetic scheme (10) according to the following rule. The number coincides with the column number, and the number of the reagent with the line number of the matrix A^T. If x_i is the initial reagent, then $a_{ij} = \alpha_{ij}$, if x_i—product, then $a_{ij} = \beta_{ij}$. If x_i is at the same time the initial reactant and the product, then $a_{ij} = \alpha_{ij} + \beta_{ij}$. Usually in an elementary stage a small amount of reagents is involved that is the stoichiometric matrix is extremely discharged.

Numerical modeling of ethane pyrolysis. The ethane pyrolysis in the absence of oxygen is described by a small sequence of stages. Ethane pyrolysis mechanism was discussed in the literature. There accepted reaction scheme offered and studied in [10]

$$C_2H_6 \rightarrow CH_3 + CH_3, \; CH_3 + C_2H_6 \rightarrow C_2H_4 + C_2H_5,$$

$$C_2H_5 \rightarrow C_2H_4 + H, \; H + C_2H_6 \rightarrow H_2 + C_2H_5, \; C_2H_5 + C_2H_5 \rightarrow C_4H_{10}.$$

Here the rate constants of stages have the form: $k_1 = 1.34 \cdot 10^{-5}$, $k_2 = 3.73 \cdot 10^2$, $k_3 = 3.69 \cdot 10^3$, $k_4 = 3.66 \cdot 10^5$ и $k_5 = 1.62 \cdot 10^7$. Let us denote the reagents concentrations as follows: $c_1 = [C_2H_6]$, $c_2 = [CH_3]$, $c_3 = [CH_4]$, $c_4 = [C_2H_5]$, $c_5 = [C_2H_4]$, $c_6 = [H]$, $c_7 = [H_2]$, and $c_8 = [C_4H_{10}]$. Then the corresponding system consists of eight ordinary differential equations of the type $C' = A^T V$, that is

$$\begin{aligned} &c_1' = -k_1c_1 - k_2c_1c_2 - k_4c_1c_6, \\ &c_2' = 2k_1c_1 - k_2c_1c_2,\ c_3' = k_2c_1c_2, \\ &c_4' = k_2c_1c_2 - k_3c_4 + k_4c_1c_6 - 2k_5c^2{}_4, c_5' = k_3c_4, \\ &c_6' = k_3c_4 - k_4c_1c_6, c_7' = k_4c_1c_6,\ c_8' = k_5c^2{}_4. \end{aligned} \tag{11}$$

The initial concentration of ethane $c_1 = [C_2H_6]$ is equal to 0.14, for the remaining reagents of concentrations it is equal to zero.

The calculations were carried out with the accuracy $\varepsilon = 10^{-2}$. The effectiveness of integration algorithms was evaluated by the number of the right side calculations if the task (11) on the integration interval. Numerical solution was carried out in the interval [0, 0.26] with the initial step $h = 10^{-5}$. This problem satisfies the "classical" definition of stiffness. At the beginning of the integration interval the transition area is observed (hundredths of a second) and then there is a slow setting. The comparison of the effectiveness of these algorithms was carried out with a known Merson method (MERSON) [11]. For all methods the actual accuracy is not worse than defined accuracy. Algorithm CESCH42 without the stability control for finding solutions required 22.853 calculations of the right side, for the algorithm with stability control CESCH42st if = 20,403, for the algorithm of variable order and step CESCH42vp the expenses are if = 2588, and for the Merson method if = 25,796.

Conclusion. From the calculation results we can conclude the following. First of all, it has been constructed the integration algorithm of the second order with the control accuracy and stability of the numerical scheme and the algorithm of variable order and step can be used to solve stiff problems. Secondly, if we take into account the computational expenditures the variable order and step algorithm CESCH42vp is nearly 10 times more efficient than the Merson method. This is a consequence of the stability control of the numerical scheme and calculations with a variable order. It appears that with the sufficiently large dimension of the problem (1) method CESCH42vp can compete with the implicit methods for problems of moderate stiffness, because it does not address the Jacobi matrix. When solving twelve test problems [2] and the ten examples [12] the advantage of the algorithm CESCH42vp is higher.

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