Adaptive Algorithm of Numerical Simulation of Stiff Dynamic Systems

Jaroslav Shmygelsky

***Abstract* — The adaptive algorithm of numerical integration of systems of the ordinary differential equations is considered. The results of numerical experiments are resulted.**

I. INTRODUCTION

The occurrence of idea about adaptive algorithms of numerical simulation of dynamic systems is closely connected to concept of a stiffness of the task. The application of an explicit method for the stiff problem, as also implicit for non stiff requires significant computing expenses.

At construction of adaptive algorithms of numerical integration it is possible conditionally to select two directions. In algorithms of the first direction depending on a degree of a stiffness of a interval of the process, which is calculated, the explicit or implicit formulas of numerical integration are applied. A classical representative of this direction is the program LSODA from the package ODEPAC, which on stiff interval uses methods BDF, and on not hard - explicit methods of Adams [1]. Let's note, that at such approach there is a number of difficulties connected to usage of diverse algorithms, in particular there is a possibility of appearance of instability on those intervals, where the explicit method in the event that a control of a local error insufficiently strict is applied.

The second group of algorithms is based on idea L.F. Shampine [2,3]. In this case implicit formulas of numerical integration are used. However on nonstiff intervals the solution of the nonlinear algebraic equations instead of a method of Newton, the method of simple iteration is applied which allows essentially to reduce computing expenses. The advantages of such approach are obvious: the problem of stability of the numerical method is completely removed, the estimation of local and global errors (and consequently also choice of a new step and a method of integration) occurs on the same procedures during all process of integration. In further the second group of algorithms is discussed.

II. BASES OF ADAPTIVE ALGORITHM

Let's consider mathematical model of the dynamic system as the ordinary differential equations:

$$\dot{\mathbf{x}} = \mathbf{f}\left(\mathbf{x}, t\right), \quad t \in [t_0, t_{\text{fin}}], \quad \mathbf{x}\left(t_0\right) = \mathbf{x}_0, \qquad (1)$$

where $\mathbf{x} \in \mathbf{R}^{\text{n}}$, $\mathbf{f}: \mathbf{R}^{\text{n}+1} \to \mathbf{R}^{\text{n}}$.

Let for numerical integration of the equation (1) the method BDF of *k*-th order is used:

$$\dot{\mathbf{x}}_{m+1} = -\frac{1}{h}\sum_{i=0}^{k} \alpha_i \mathbf{x}_{m+1-i}, \quad 0 \le k \le 6. \qquad (2)$$

Discrete model of the system (1) at application of a method (2) can be represented as:

$$\mathbf{x}_{m+1} = -\frac{h}{\alpha_0}\mathbf{f}\left(\mathbf{x}_{m+1}, t_{m+1}\right) + \mathbf{d}, \quad m = 0,1,2,\ldots, \qquad (3)$$

where $\mathbf{d} = -\frac{1}{h}\sum_{i=1}^{k} \alpha_i \mathbf{x}_{m+1-i}$ - vector, which does not depend from $\mathbf{x}_{m+1}$.

The equation (3) is usually solved on each step by a method of Newton or its modification. On this procedure a main volume of computing expenses are wasted.

Let's write a method of simple iteration for solution of the equation (2):

$$\mathbf{x}_{m+1}^{i+1} = -\frac{h}{\alpha_0}\mathbf{f}\left(\mathbf{x}_{m+1}^{i}, t_{m+1}\right) + \mathbf{d}, \quad i = 0,1,2,\ldots \qquad (4)$$

The method (4) locally converges to solution $\mathbf{x}_{m+1}$, if in some vicinity of this solution containing initial approximation $\mathbf{x}_{m+1}^{0}$, condition:

$$\frac{h}{\alpha_0}\left\|\mathbf{f}'\left(\mathbf{x}_{m+1}, t_{m+1}\right)\right\| \le q < 1, \qquad (5)$$

is satisfied, where $\|\cdot\|$ - any matrix norm. It is clear, that at good convergence of a method of simple iteration the computing expenses on one step will be close to expenses, which arise at usage for numerical integration of the system (1) explicit methods.

For support of satisfactory convergence of a method of simple iteration the value of *q* should not exceed 0,5, that usually takes place on non stiff intervals of an integral curve owing to small values of step h. Therefore condition (5) at $q \le 0,5$ can be used for criterion of transition from a method of Newton to a method of simple iteration [3].

The hard limitations on convergence of a method of simple iteration reduce efficiency of similar algorithms a little. Therefore in [4] it is offered at

Author are with the Lviv National University named by Ivan Franko, Tarnavsky str. 107, 79017 Lviv, Ukraine, e-mail: *shmygelsky@rd.wups.lviv.ua*

solution of the system (5) to apply a method of the generalized iteration:

$$\mathbf{x}_{m+1}^{i+1} = \mathbf{x}_{m+1}^{i} - \mathbf{D}\left(\mathbf{x}_{m+1}^{i} + \frac{h}{\alpha_0}\mathbf{f}\left(\mathbf{x}_{m+1}^{i}, t_{m+1}\right) - \mathbf{d} \right), \quad i = 0,1,2,..., \tag{6}$$

from which the matrix D is selected so that the iterative procedure (6) converged at the large values of step h, than method of simple iteration. The elementary case, if $\mathbf{D} = \beta\mathbf{I}$, где β - some scalar, $\mathbf{I}$ – unit matrix. Then:

$$\mathbf{x}_{m+1}^{i+1} = (1-\beta)\mathbf{x}_{m+1}^{i} - \beta\left(\frac{h}{\alpha_0}\mathbf{f}\left(\mathbf{x}_{m+1}^{i}, t_{m+1}\right) - \mathbf{d} \right), \quad i = 0,1,2,... \tag{7}$$

At $\beta = 1$ we have a method of simple iteration (4). For the extension of area of convergence of a method (7) in comparison with a method of simple iteration it is necessary to keep a condition: $|\beta| < 1$ [4]. Where decreases β the convergence domain increases, but the speed of convergence becomes unsufficient. Therefore optimal choice of values q и β has the large significance for effective operation of adaptive algorithm.

III. NUMERICAL EXPERIMENTS

The results of numerical experiments are given below in which there were compared the speed of three programs of numerical integration of the ordinary differential equations: BDFR, BDFRA and RKDP54.

On a basis of programs BDFR and BDFRA the variant of a method BDF with differences of the maximum orders and effective procedures of choice of an integration step and about a method from 1-st up to 6-th. In the program BDFR the system of the nonlinear equations (2) on each step is solved by a method of Newton. In programs BDFRA on non stiff intervals for this purpose was used a method (7). The transition from a method of Newton to a method (7) (i.e. definition of a non stiff intervals of a trajectory) occurs at execution of criterion (5). The return transition to a method of Newton is carried out when the method (7) does not converge for three iterations. The program RKDP54 is based on methods of Runge-Kutta 5-4 orders in formulation of Dorman-Prince. In opinion of the experts this method is the best for the problems with a small and average degree of a stiffness, if the low accuracy of calculation (10^{-3}-10^{-6}) is necessary [5].

The comparison was carried out on the nonlinear system of 20 order, which consists of 10 uncoupled equations of Van-der-Pol:

$$\begin{aligned} \dot{x}_i &= x_{i+1} \\ \dot{x}_{i+1} &= \varepsilon \cdot \left(1 - x_i^2\right) \cdot x_{i+1} - x_i, \quad i = 2j-1, \ j = \overline{1,10} \end{aligned} \tag{8}$$

It is known that equation of Van-der-Pol is one of the most successful tests for check of practical algorithms. With the help of the parameter ε it is possible easily to change a stiffness of the system. Besides the eigenvalues of a matrix Jacobi along solution vary in very wide ranges, passing from real to complex and contrary.

The system (8) was integrated on a interval $[0, t_{\text{fin}}]$ from the initial conditions $x_i(0) = 2$, $x_{i+1}(0) = 0$ at different values ε and t_{fin}. The boundary of a local error of discretization on step for all programs was equal 10^{-4}. The accuracy of solution of the equations (2) for programs BDFR and BDFRA was equal to 10^{-5}. In the program BDFRA for criterion (3) it was necessary q=0,4. . The calculation were carried out on the personal computer with low speed, that the run time was appreciable. The results of numerical experiments are given in the table.

The program	Run time (s)			
	$\varepsilon = 1$, t_{fin}=20	$\varepsilon = 20$, t_{fin}=40	$\varepsilon = 50$, t_{fin}=100	$\varepsilon = 100$, t_{fin}=200
BDFR	111,98	98,47	109,80	122,43
BDFRA (ß=1)	26,25	47,51	62,18	72,17
BDFRA (ß=0,7)	27,78	43,67	52,61	61,79
RKDP54	6,98	36,86	179,44	716,87

IV. CONCLUSIONS

As the results of numerical experiments adaptive algorithms at all degrees of a stiffness of the problem work much faster, than classical implicit methods, and at small and average stiffness can successfully compete with explicit methods.

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