Parallel time step control of lines method for the evolution equations

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The problems of obtaining solutions for partial differential equations with the help of the method of lines are considered, which is a semi-discrete method with discretization over spatial variables. Such an approach made it possible to effectively implement a large class of evolutionary equations. The problems of solving the received SODEs by collocation block methods are considered, allowing to provide an effective parallel implementation. Moreover, all the advantages of the solution (parallel step control, local error control, stability of the solution) are realized for the case of partial derivatives without significant increase in computational complexity.

Keywords — evolution equations, method of lines, Cauchy problem, parallel step control, block methods, τ-refinement

I. Introduction

In this work, the main attention is focused on the control of the step of integration over time (τ-refinement) in the realization of the method of lines for partial differential equations by collocation block difference schemes. The method of straight lines [1-2] for simplicity of presentation is considered using the example of a one-dimensional parabolic equation and is a semi-discrete method with discretization in terms of spatial variables, ensuring the reduction of the original evolution equation with partial derivatives

$$\frac{\partial u}{\partial t} = a^2 \frac{\partial^2 u}{\partial x^2} + f(x,t), x \in [x_0, \mathrm{L}], \quad t \in [t_0, T] \qquad (1)$$

with initial condition of the form

$$u(x, t_0) = q(x), \qquad (2)$$

boundary conditions of the first, the second or the third kind of Cauchy problem

$$u' = \varphi\big(t, u(t)\big), u(t_0) = u_0, t \in [t_0, T], \qquad (3)$$

described by a system of ordinary differential equations (SODE). Such an approach allows us to effectively implement a large class of evolutionary equations. However, after reducing the partial differential equation to the Cauchy problem for SODE, problems arise that were not characteristic of the original problem. So, if we consider explicit implementation patterns, then the choice of the step of integration over time is determined by the fulfillment of the Courant condition [3] and directly depends on the step size over the spatial variable. For the case of implicit difference schemes, the time step is regulated by the physical nature of the problem being solved and the order of approximation of the difference scheme(s).

When it comes to numerical solution of the generated ODEs system, additional possibilities arise related to approximation of higher order (p-refinement), local error control and automatic change of integration step (τ-refinement). A significant influence on the error of the resulting solution will also be provided by questions related to the step change over the spatial variable (h-refinement). However, in this case, a simple reduction of the spatial step by a certain coefficient γ leads to an increase in the dimension of the formed SODE by the same coefficient, which considerably complicates the solution. Therefore, in this section we will consider questions related only to τ-refinement, which is especially important for the numerical solution of rigid differential equations. At the same time, the issues of correlating the errors of the results and the time spent on obtaining the solution are relevant.

II. Controlling the step on collocation schemes when implementing evolution equations by the method of lines

The approaches considered in [4-5], connected with the control of the local error based on the comparison of solutions obtained with different orders in coinciding points of the block, is very effective in solving non-rigid equations and systems and can be used to estimate the error of the solution obtained. If we obtain a priori estimates of the integration step to ensure a given accuracy before the count begins, then it can be asserted that in any part of integration the error obtained does not exceed the specified error. But, unfortunately, this approach cannot provide a change in the integration step at the time of invoice. This question becomes most relevant when the desired function (s) at individual areas of integration is characterized by different rates of change. In this case, it is advisable to use the adaptable step for integration, which does not allow to provide the calculated collocation schemes [6]. To eliminate this drawback, new calculation schemes can be introduced, which will also be based on interpolation polynomials whose degrees coincide with the number of collocation points, and the values of the polynomials at these points coincide with the right-hand sides of the differential equation at the calculated points [5-6]. But the collocation points do not necessarily have to be a uniform grid, although it is desirable (but not necessary) that they be related to each other by some proportionality factors, for example, powers of two. Since it is a question of multi-step methods, it is necessary to select a set of points forming a support block

$$t_{n,i} = t_{n,0} + i\tau_n \in \left[t_{n,-m+1}, t_{n,0}\right], \quad i = -(m-1), -(m-2), \dots, 0,$$

as well as two sets of points that will form the calculation blocks

$$t_{n,i}^{(1)} = t_{n,0} + i\tau_{n_1} \in [t_{n,0}, t_{n,s_1}], i = 1,2, \dots, s_1,$$

$$t_{n,i}^{(2)} = t_{n,0} + i\tau_{n_2} \in [t_{n,0}, t_{n,s_2}], i = 1,2, \dots, s_2.$$

The simplest way to do this is to associate the integration steps τ_{n_1} and τ_{n_2} with the relations $\tau_{n_1} = 2\tau_{n_2}$. Then the dimensions $s_2 = 2s_1$. should be fulfilled between the dimensions of the calculated blocks. The account, as in the previous case, will be executed in parallel for two computational schemes with the same dimensions of the reference blocks and with the dimensions of the calculated blocks that differ in s_2/s_1 times. The canonical form of multi-step collocation methods with the number of reference points *m* and the number of calculated points s_1 and s_2, respectively, will have the form

$$u_{n,i}^{(1)} = u_{n,0} + \tau_n \sum_{j=1-m}^{0} b_{i,j}^{(1)} F_{n,j} + \tau_{n_1} \sum_{j=1}^{s} a_{i,j}^{(1)} \ F_{n,j}^{(1)},$$

$$i = 1,2, \dots, s_1, \qquad (4)$$

$$u_{n,i}^{(2)} = u_{n,0} + \tau_n \sum_{j=1-m}^{0} b_{i,j}^{(2)} F_{n,j} + \tau_{n_2} \sum_{j=1}^{s} a_{i,j}^{(2)} \ F_{n,j}^{(2)},$$

$$i = 1,2, \dots, s_2,$$

where $u_{n,i}^{(1)}, u_{n,i}^{(2)}$ – are approximate values of the solution of the Cauchy problem (3) at the points $t_{n,i}^{(1)}, t_{n,i}^{(2)}$ respectively,

$\tau_n, \tau_{n_1}, \tau_{n_2}$ – are the steps of integration in the reference block, in blocks of dimension s_1 and s_2, respectively,

$F_{n,j} = \varphi(t_n + j\tau, u_{n,j})$ – are the right-hand sides of the equation (3) at the points, $j = -(m-1), -(m-2), \dots, 0,$

$F_{n,j}^{(1)} = \varphi(t_n + j\tau_{n_1}, u_{n,j}), j = 1,2, \dots, s_1,$

$F_{n,j}^{(2)} = \varphi(t_n + j\tau_{n_2}, u_{n,j}), j = 1,2, \dots, s_2,$

$a_{i,j}^{(1)}, b_{i,j}^{(1)}, a_{i,j}^{(2)}, b_{i,j}^{(2)}$ – coefficients of the design schemes (4).

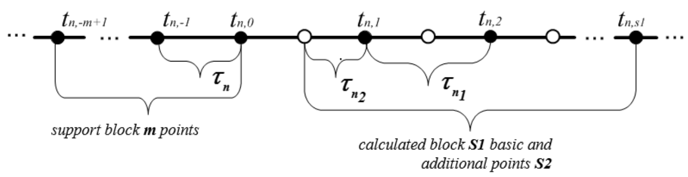

Fig. 1. Scheme of fixing the reference, calculated and intermediate points

To delineate the calculated and sought-for points, appropriate notation and representation of them in the vector form were implemented.

$U_n = \{u_{n,j}\}, \ n = 1,2, \dots, \ j = -(m-1), -(m-2), \dots, 0$ – the vector of counted points,

$U_{n+1} = \{u_{n,j}\}, \ n = 1,2, \dots, \ j = 1,2, \dots, s_1$ – the vector of the required points for the dimension of the block s_1,

$V_{n+1} = \{u_{n,j}\}, \ n = 1,2, \dots, \ j = 1,2, \dots, s_2$ – is the vector of the desired points for the dimension of the block s_2,

$F_{n,j} = \varphi(t_n + j\tau_n, u_{n,j}), \ n = 1,2, \dots, \quad j = -(m-1), -(m-2), \dots, 0,$

$F_{n+1,j} = \varphi(t_n + j\tau_{n_1}, u_{n,j}), n = 1,2, \dots, j = 0, 1, \dots, s_1,$

$\Psi_{n+1,j} = \varphi(t_n + j\tau_{n_2}, u_{n,j}), \ n = 1,2, \dots, j = 0, 1, \dots, \ s_2$ – respectively, the right-hand sides of equation (6) at known and sought-for points,

$A^{(1)}, B^{(1)}, A^{(2)}, B^{(2)}$ – are the matrices of the coefficients of the difference schemes,

$U_{n,0} = (u_{n,0})e$ – is the solution at the point $t_{n,0}$,

e – is a unit vector of dimension *s*.

Then in vector form the system of equations (4) for the case under consideration will have the following form

$$U_{n+1} = U_{n,0} + \tau_n B^{(1)} F_n + \tau_{n_1} A^{(1)} F_{n+1}, \qquad (5)$$

$$V_{n+1} = U_{n,0} + \tau_n B^{(2)} F_n + \tau_{n_2} A^{(2)} \Psi_{n+1}.$$

To begin the calculation, it is necessary to enter a set of reference values, which can be determined by a one-step method that provides the required accuracy of calculations. Then the search for a numerical solution can be reduced to a solution at each step of two nonlinear systems of equations (5), with a sequential definition of the vectors $U_1, V_1, U_2, V_2 \dots$ After determining the unknown coefficients and forming the matrices $A^{(1)}, B^{(1)}$ with dimensions $s_1 \times m$ and $s_1 \times s_1$, $A^{(2)}, B^{(2)}$ with dimensions $s_2 \times m$ and $s_2 \times s_2$, computations by a multi-step block method represented in the form of systems (5) can be reduced to the following iterative processes

$${U_{n+1}}^{(1)} = U_{n,0} e + \tau_n B^{(1)} F_n, \qquad (6)$$

$${U_{n+1}}^{(r+1)} = (U_{n,0} e + \tau_n B^{(1)} F_n) + \tau_{n_1} A^{(1)} {F_{n+1}}^{(r)},$$

$$n = 1,2, \dots, r = 1,2, \dots s_1,$$

$${V_{n+1}}^{(1)} = U_{n,0} e + \tau_n B^{(2)} F_n,$$

$${V_{n+1}}^{(r+1)} = (U_{n,0} e + \tau_n B^{(2)} F_n) + \tau_{n_2} A^{(2)} {\Psi_{n+1}}^{(r)},$$

$$n = 1,2, \dots, r = 1,2, \dots s_2.$$

The systems in (6) require preliminary determination of the values of the vector U_0 at the reference points of the initial block. Determination of the initial values ${U_{n+1}}^{(1)}$, ${V_{n+1}}^{(1)}$ in the calculation blocks is carried out on the basis of the multi-step predictor method of Adams, which allows increasing the accuracy of the initial approximation. The computation of the approximate values ${U_{n+1}}^{(r+1)}, {V_{n+1}}^{(r+1)}$ of the solution of the Cauchy problem in each next computation block is carried out iteratively and independently. After obtaining the solution in the next block, the obtained values are compared in coinciding points. The magnitude of the norm of the discrepancy between the values of approximate solutions in the coinciding s_1 nodes of the main block is decisive for deciding on the step size.

Just as in the formation of multi-stage collocated block difference schemes, which are used to solve the initial Cauchy problem, when reducing equations (1), for controlling the integration step, it is necessary to first build several calculation schemes, namely: basic design schemes corresponding to integration with unchanged step, as well as the schemes to which the calculation will be transferred in case of providing an increase or reduction of the step. In this case, the steps for increasing the step (stretching) will characterize the changes only in the calculation block, and the reduction schemes will make changes both to the design and reference blocks. In fact, the generation of these schemes is reduced to the determination of the calculation coefficients and is carried out once, before the beginning of the calculations, implying their repeated use in solving various problems. For each type of difference schemes, the developed software system allows determining the maximum order of approximation and estimating the a priori error value at the nodes of the calculation block.

III. Numerical Realization of the Method of Lines with Variable Time Step Control (T-Refinement)

Experiments to control the step of integration with respect to the time variable (τ-refinement) were carried out for different values of the discretization step in space, based on the value of (h-refinement), the number of equations n in the SODEs (n=10, n=20, n=40). For test problems with a known exact solution, exact values were used to form values at m initial points. For cases where there was no exact solution, the required sets of initial values were determined by a one-step method with comparable accuracy. As the initial approximations $F_{n,1}, F_{n,2}, \dots, F_{n,s}$, the values calculated with the help of the predictor Adams [7] were used for the next calculation block. In conducting numerical experiments, in addition to the main indicators, the ratio of the number of effective steps to the total number of counts was also estimated.

Test problem 1. The already known test problem [8] (1) with initial condition

$$u(x,0) = sin(\pi x) + \sin(k\pi x), \qquad (7)$$

boundary conditions of the first kind

$$u(0,t) = u(L,t) = 0, \qquad (8)$$

with known exact solution

$$u(x,t) = e^{-\pi^2 a^2 t} sin(\pi x) + e^{-\pi^2 a^2 k^2 t} sin(k\pi x)$$

was considered as experimental. As the stiffness parameter, the values $k = 1,2, \dots ,10$.

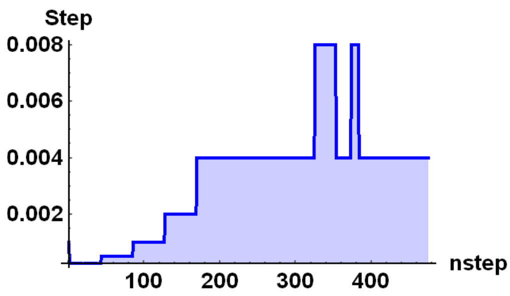

Fig. 2. Automatic change of the integration step for the problem (1, 7-8), $n = 10,\ k = 2, \varepsilon = 10^{-6}$

As shown in [8], methods without step control for such values of the parameter $k > 1$ cannot provide the declared accuracy of the calculation. In fig. 2-3 graphs of step change in time variable, obtained during the implementation of the test task using the system of difference schemes (6) with the dimensions of the reference and calculation blocks 2×2 and 2×4 are constructed.

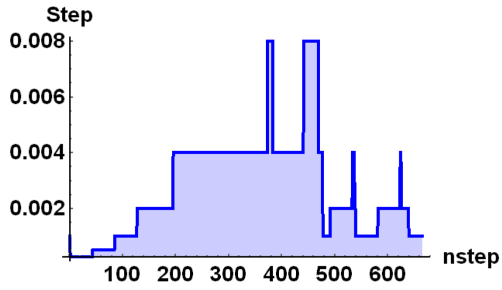

Fig. 3. Automatic change of the integration step for the problem (1, 7-8), $n = 10,\ k = 10, \varepsilon = 10^{-6}$

The dynamics of the step change was also investigated depending on the discretization step in space, the stiffness parameter k, which took values in the interval 1 ÷ 10, and the value of the given global error ε.

Test problem 2. The test was performed for a parabolic equation with the known exact solution described in [9]. We consider a special case of the heat equation (1) with the values of the parameters $L = 1, T = 1, a = 1$, with the initial condition

$$u(x,0) = sin(\pi x/L), \qquad (9)$$

boundary conditions of the first kind (8), and the known exact solution

$$u(x,t) = e^{-\left(\pi^2/L^2\right)t} sin\left(\frac{\pi x}{L}\right).$$

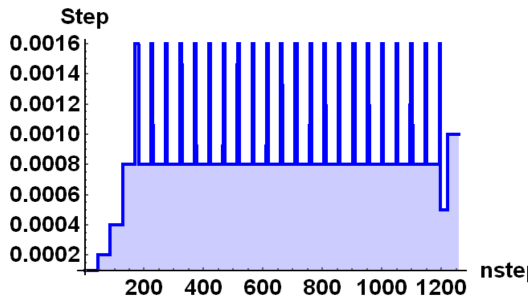

Fig. 4. Automatic change of the step for the problem (1, 8-9) in the method of lines, $n = 10, \varepsilon = 10^{-6}$

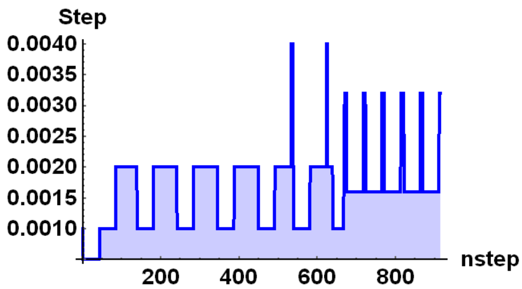

Fig. 5. Automatic change of the step for the problem (1, 8-9) in the method of lines, $n = 20, \varepsilon = 10^{-6}$

The experiment is aimed at conducting a comparative analysis of the results of numerical implementation using direct ones with an exact solution. The dynamics of the step change was investigated depending on the discretization step in space $h = L/n$, which determined the dimension of the system of ordinary differential equations $n = 10, 20, 40$. Different consequences of global error ε were set. The method of lines was realized using difference schemes (6) with reference and calculation dimensions 2×2 (2×4) and 3×3 (3×6) (fig. 4-5).

Test problem 3. Testing was carried out for the test problem Schisser [9]. We consider the heat equation (1) over space intervals $-5 \le x \le 5$ and in time $0 \le t \le 1$, with the parameter $a = 1$, using the initial condition

$$u(x,0) = \frac{1}{2} e^{-(x-1)^2} + e^{-(x+2)^2}, \tag{10}$$

with the known exact solution, with the boundary conditions on the left-Dirichlet and on the right-Neumann

$$u(-5,t) = 0,\ \ \partial u(5,t)/\partial x = 0. \tag{11}$$

The dimension of the system of ordinary differential equations for the method of lines was chosen for the values $n = 10, 20, 40$. These values of n determined the discretization step with respect to the space $h = L/n$. The value of the global error ε was set at the level $\varepsilon = 10^{-6}, \varepsilon = 10^{-9}$. To implement the method of lines, difference schemes (6) with dimensions of the reference and computational blocks 2×2 (2×4) and 3×3 (3×6) were used. The results of numerical simulation are presented in the form of step change diagrams (fig. 6).

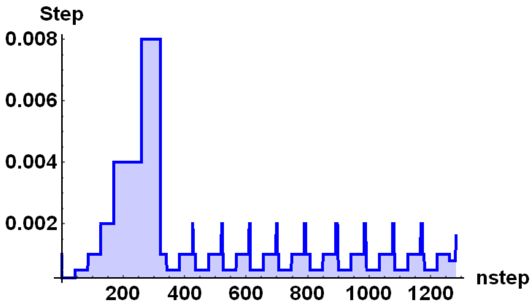

Fig. 6. Automatic change of the integration step for the problem (1, 10-11) in the method of lines, $n = 20, \varepsilon = 10^{-6}$

In all the model experiments performed for this task, in addition to the requirements for retaining a given error, indicators were monitored that ensure the decision to change the step size (the inertia parameter, the number of iterations to refine the solution by the Newton method, the closeness of the current local error to the limit value, effective steps to the total number of counted, etc.). The obtained results testify to the high effectiveness of the proposed approach, which is based on the use of multi-step collocation block schemes with variable dimensions of support blocks and calculation blocks for automatic step control (τ-refinement) in the method of lines.

IV. Conclusions

The investigations carried out in this section have made it possible to propose new approaches to solving the problem of parallel control over the step of integration over a variable time in the realization of the method of lines for partial differential equations by collocation block difference schemes. For controlling the time variable step in evolution equations is based on the use of multi-step multi-point collocation block schemes with uneven arrangement of nodes connected by some proportionality coefficients. When modeling with the help of such schemes, the local error of numerical integration was estimated as the norm of the discrepancies of the solutions obtained with different order of approximation at coinciding points of the computational blocks. The value of the received error and the state of the values of the indicators were used to decide on the size of the next step in the variable time. This made it possible to provide the specified accuracy at each site. If it is necessary to shorten the step length, in the calculation schemes, the previously calculated values were used as intermediate ones, which made it possible to significantly reduce the number of computational operations.

For the automatic generation of computing circuits, a software system based on the use of the integro-interpolation method has been developed, which makes it possible to generate the coefficients of difference equations with arbitrary dimensions of computational and reference blocks, with the possibility of transition to stretching-step compression schemes. The numerical solution for each calculation block was carried out by means of an iterative process, to accelerate the convergence, the initial approximations were determined using the Adams predictor method. The theoretical positions given in the paper are supported by experimental studies on test problems with known exact solutions.

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