ALGORITHM FOR INCREASING THE ACCURACY OF A NUMERICAL SOLUTION OF THE EQUATIONS OF MATHEMATICAL PHYSICS BY THE GAUSS–LEGENDRE METHOD OF QUADRATURES

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UDC 519.615.62

An effective algorithm is developed for increasing the accuracy of a numerical solution of the equations of mathematical physics. In the first stage of the algorithm, with the aid of a stable method, values of the unknown function are calculated at the nodes corresponding to the Gauss–Legendre quadratures (GLQ). In the second stage recalculation is carried out in accordance with the GLQ formulas.

A method for integrating ordinary differential equations (ODE) by means of Gauss–Legendre quadratures possessing the highest algebraic degree of accuracy was considered previously in [1], but, in its time, did not find wide practical application. In the present paper, with the aim of increasing the accuracy of a numerical solution of the equations of mathematical physics, we propose to use the GLQ method in combination with some stable method of low order of accuracy. In this connection, the calculations are carried out in two stages. In the first stage, using the stable method selected, approximate values of the unknown function are obtained at the nodes of an auxiliary grid corresponding to the GLQ. In the second stage a recalculation is carried out according to the GLQ formulas. We show, as a result of introducing such a procedure, that the accuracy of the final result is increased.

The method for increasing the accuracy of a numerical solution of the equations of mathematical physics using the GLQ formulas is tested on a series of Cauchy problems for first order ODE and on a second boundary value problem for the heat conduction equation.

1. Increasing the Order of Accuracy of an Approximate Solution of a Cauchy Problem for a First Order ODE. Let us assume that it is required to find a function u(t), continuous for $t_0 \leqslant t \leqslant t_j$, satisfying the differential equation

$$\frac{du}{dt} = f(u,\ t) \tag{1}$$

and the initial condition

$$u(t_0) = u_0. \tag{2}$$

We assume that the solution of problem (1)-(2) exists and is unique, i.e., we assume that all the conditions of an appropriate theorem guaranteeing the existence and uniqueness of a solution of a Cauchy problem (see [2]) are satisfied.

On the interval $[t_0,\ t_f]$ we introduce a uniform grid with integral nodes

$$t_k = t_0 + k\tau, \tag{3}$$

where k = 0, 1, 2, ..., N; $\tau = (t_f - t_0)/N$ is the grid step. We also introduce an auxiliary nonuniform grid with nodes defined by the relations

$$t_{ki} = t_k + \tau\theta_i, \tag{4}$$

where i = 1, 2, ..., n; θ_i are the GLQ nodes [3].

We assume that on the auxiliary grid $\{t_{ki}\}$ the grid function y_{ki} is found with the aid of some stable method, this function being an approximate solution of the Cauchy problem (1)-(2), whereby the maximum error does not exceed some quantity ε_1 in absolute value.

We integrate equation (1) in a strip from t_k to t_{k+1}:

$$u_{k+1} = u_k + \int\limits_{t_k}^{t_{k+1}} f(u,\ z)\,dz, \tag{5}$$

Brest Structural Engineering Institute. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 55, No. 2, pp. 299-304, August, 1988. Original article submitted April 23, 1987.

 0022-0841/88/5502-0930$12.50

where u_k is the exact value of the unknown function at the node t_k. Relation (5) is exact as long as we do not apply to the integral on the right side a quadrature formula for its numerical integration, each such formula generating a specific computational process. Applying the GLQ formulas to equation (5), for a recalculation we obtain

$$y_{k+1} = y_k + \tau \sum_{i=1}^{n} \omega_i \tilde{f}_{ki}, \tag{6}$$

where $\tilde{f}_{ki} = f(y_{ki}, t_{ki})$ are approximate values of the right side of equation (1); ω_i are the GLQ weights [3], and y_k is a grid function giving an approximate solution of the Cauchy problem (1)-(2) on the uniform grid.

We show that the application of formula (6) makes it possible to increase the order of accuracy of the intermediate result. Since y_{ki} is determined in the first stage with an error not exceeding ε_1 in absolute value,

$$y_{ki} = u_{ki} \pm \varepsilon_1, \tag{7}$$

it follows that f_{ki} is determined from formula (7) with error not exceeding some quantity ε_2. Consequently,

$$f_{ki} = \tilde{f}_{ki} \pm \varepsilon_{ki}, \tag{8}$$

where $f_{ki} = f(u_{ki}, t_{ki})$ are the exact values of the right side of equation (1), obtained by substituting into it the exact values of the unknown function

$$u_{ki} = u(t_{ki}) \tag{9}$$

at the nodes corresponding to the GLQ, and the ε_{ki} are the errors determined by equation (8). Substituting $\tilde{f}_{ki}$ from equation (8) into equation (6), we obtain

$$y_{k+1} = y_k + \tau \sum_{i=1}^{n} \omega_i f_{ki} + \tau \sum_{i=1}^{n} \omega_i (\pm \varepsilon_{ki}). \tag{10}$$

Since, by definition, ε_{ki} does not exceed ε_2, we can represent the remainder in formula (10) in the form

$$R_{ki} = \tau \sum_{i=1}^{n} \omega_i (\pm \varepsilon_{ki}) \leqslant \tau\varepsilon_2. \tag{11}$$

We have here used the fact that (see [4])

$$\sum_{i=1}^{n} \omega_i = 1. \tag{12}$$

Thus we obtain the following estimate for equation (10):

$$y_{k+1} = y_k + \tau \sum_{i=1}^{n} \omega_i f_{ki} + \tau\varepsilon_2. \tag{13}$$

The appropriateness of applying the given algorithm depends, consequently, on the relationship of the quantities ε_1, ε_2, and τ. In this case it is appropriate to apply the algorithm if the following relationship is satisfied:

$$\varepsilon = \tau\varepsilon_2 < \varepsilon_1. \tag{14}$$

Starting from the condition (14), we can easily determine the step size τ guaranteeing the required accuracy ε.

Remark. The error of the GLQ method itself, arising due to approximating the integral in equation (5) by the finite sum in equation (6), is readily determined from well-known formulas [4] and is not considered here on the assumption that it can be made less than that in relation (14) by choosing the number of nodes in the GLQ.

2. Solution of the Second Boundary Value Problem for the Heat Conduction Equation by the GLQ Method. We consider the second boundary value problem for the linear normalized heat conduction equation in temperature form

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad 0 \leqslant x \leqslant 1, \tag{15}$$

with boundary conditions

$$\left.\frac{\partial u(x,t)}{\partial x}\right|_{x=0} = \varphi(t), \quad \left.\frac{\partial u(x,t)}{\partial x}\right|_{x=1} = \psi(t) \tag{16}$$

and initial condition

$$u(x,0) = u_0(x) \tag{17}$$

It was shown in [6] that a numerical solution of the second boundary value problem in the temperature form (15)-(17) is nonconservative, i.e., it does not satisfy the discrete analog of the conservation law for energy. It was shown there that a transition to the flux form makes it possible to eliminate this shortcoming. The appropriate transition is effected by introducing the heat flow function

$$W(x,t) = \frac{\partial u(x,t)}{\partial x}. \tag{18}$$

Equation (15) and conditions (16)-(17) are thus transformed to the following form:

$$\frac{\partial W}{\partial t} = \frac{\partial^2 W}{\partial x^2}, \tag{19}$$

$$W(0,t) = \varphi(t), \quad W(1,t) = \psi(t), \tag{20}$$

$$W(x,0) = \frac{\partial u_0(x)}{\partial x}. \tag{21}$$

The boundary value problem of the second kind becomes thereby a boundary value problem of the first kind relative to the function W(x, t). To solve the problem (19)-(21) by the method of finite differences, one can choose, for example, an implicit scheme with weights [5] or the method of asymmetric difference schemes (ASD), described in [7] for the Burgers equation and in [8] for a quasilinear heat conduction equation. An algorithm was presented in [9] for restoration of the conservative property of the difference schemes, violated, as shown in [6], when difference equations are solved by iterational methods. Moreover, the ASD method possesses an algorithmic structure suitable for use on a multiprocess computer, since, in contrast to the driver method, the ASD method does not require the preliminary procedure of transforming a sequential algorithm into a parallel type.

As we did in Sec. 1 we introduce two grids. A uniform grid with equidistant nodes: $x_i = ih$; $i = 0, 1, 2, \ldots, N-1$; $h = 1/N$; $t_k = t_0 + k\tau$; $k = 0, 1, \ldots, K$; $\tau = (t_f - t_0)/K$, and an auxiliary grid, nonuniform with nonequidistant nodes along the spatial coordinate: $x_{ij} = x_i + h\theta_j$, $j = 1, \ldots, n$. It should be noted that distances between two arbitrary neighboring nodes of the auxiliary grid having a fixed index j are identical and equal to h. Consequently, the nonuniform grid $\{x_{ij}, t_k\}$ introduced in this way can be represented in the form of a set of n uniform grids $\{x_i, t_k\}_j$, shifted in space along coordinate x, one relative to another, by an amount equal to $h\theta_j$. Thus, a calculation on each of the uniform grids with a shift of $\{x_i, t_k\}_j$ can be made from formulas with a constant step, except for two intervals of partition along the spatial coordinate x: the first and the last. Steps h_{1j} and h_{Nj} differ from h and are calculated as follows: $h_{1j} = h\theta_j$, $j = 1, \ldots, n/2$; $h_{Nj} = h\theta_j$, $j = n/2 + 1, \ldots, n$.

Let us assume that the boundary value problem (19)-(21) has been solved by one of the methods selected on the nonuniform grid $\{x_{ij}, t_k\}$, i.e., the grid function W_{ij}^k has been found. We integrate equation (18) with respect to the time t from $t_{k-1/2}$ to $t_{k+1/2}$, and with respect to the coordinate x from x_i to x_{i+1}. We now apply the GLQ method to the resulting integral. As a result, we obtain formulas for the transition from the calculated values of the flows to the values of the temperature:

$$u_{i+1}^k = u_i^k + h\sum_{j=1}^{n} \omega_j W_{ij}^k. \tag{22}$$

It is easy to show, as in the case of ODE, that the order of accuracy of the final result is increased thereby.

3. Verification of the Effectiveness of the Procedure for Integrating ODE by the GLQ Method. With a systematic procedure we solved the following Cauchy problems:

$$y' = \pm y,\ \ y(0) = 1,\ \ y(t) = \exp(\pm t); \tag{23}$$

$$y' = t - y,\ \ y(0) = 0,\ \ y(t) = t - 1 + \exp(-t); \tag{24}$$

$$y' = 2xy,\ \ y(0) = 1,\ \ y(t) = \exp(t^2); \tag{25}$$

$$y' = y\,\mathrm{tg}\,t + \cos t,\ \ y(0) = 1,\ \ y(t) = \left(\frac{2+t}{\cos t} + \sin t\right)\Big/ 2; \tag{26}$$

$$y' = y^2 + 1,\ \ y(0) = 0,\ \ y(t) = \mathrm{tg}\,t. \tag{27}$$

The integration step τ in all cases was taken to be 0.1. For problems (23)-(26) the interval of variation for t was $0 \leqslant t \leqslant 1$; for problems (27) it was $0 \leqslant t \leqslant 1.5$.

For obtaining an approximate solution at the nodes of the auxiliary grid we chose, in the first stage, a stable method for integrating ODE, one which allowed us to easily vary the step size in the computational process [10]. In the second stage we applied the GLQ method with the number of nodes n = 2. A comparison of the intermediate and final solutions with the known analytical solutions allowed us to make a statement concerning the increase in accuracy of the final result compared with the intermediate result.

4. Results of the Numerical Solution by the GLQ Method of a Boundary Value Problem of the Second Kind for the Heat Conduction Equation. To verify the effectiveness of the method chosen for solving problems (15)-(17) the following boundary and initial conditions were selected: $\varphi(t) = \psi(t) = 0$ and $u(x, 0) = 1 + \cos \pi x$. An analytic solution exists for this case, given by

$$u(x, t) = 1 + \exp(-\pi^2 t)\cos \pi x. \tag{28}$$

Problem (15)-(17) was solved systematically with specified accuracy using the standard subroutine PKG2 (see [11]), appropriate for the solution of both linear and nonlinear boundary value problems of mathematical physics of the second kind. A comparison of the numerical solution obtained using the standard subroutine PKG2 with the analytical solution (28) showed that the specified accuracy was attained only at the center of the interval of integration [0, 1] with the steps $\tau = h = 0.1$. At the ends of this interval the residual turned out to be rather substantial. The same type of situation (with nonessential differences) proved to be typical also for the solution of the boundary value problem (19)-(21) by the driver method using an implicit scheme with weights [5]. In this case the following conditions were selected: $W = (0, t) = W(1, t) = 0$ and $W(x, 0) = -\pi \sin \pi x$. Transition from flow values to temperature values was effected in accord with the following formula [6]:

$$u_i^{n+1} = u_i^k + \tau (W_{i+1}^{k+1} - W_i^{k+1})/h. \tag{29}$$

Solution of problem (19)-(21) by the GLQ method showed that the residual, after a recalculation in accordance with formula (22), decreased. It should be noted that in applying formula (22) one needs to know at least one value of the temperature on the upper layer with respect to the time. In this case it is convenient to apply, for example, the method used in [6].

The algorithm for increasing the accuracy of a numerical solution by means of the GLQ method can also be extended even to nonlinear equations of mathematical physics involving partial derivatives. In particular, we propose, in subsequent work, to use the GLQ method for the numerical solution of a nonlinear dynamic problem from the theory of thermoelasticity since in attempting to solve a connected system involving the parabolic equation of heat conduction and the hyperbolic equation of thermoelasticity by the standard finite differences method [11] it was observed that the nature of the behavior of the thermal stress field depended very strongly on the accuracy of approximation of the temperature field.

NOTATION

t_0, initial time instant; t, time; t_f, final time instant; u(t), unknown function in analytical solution; y(t), unknown function, numerical solution; f(u, t), known function of u and t; u_0, initial condition; τ, time step; N, number of subdivisions of interval of integration; θ_i, values of the GLQ nodes; y_{ki}, approximate solution of Cauchy problem on auxiliary nonuniform grid; ε_1, maximum error of approximate solution at the first stage; ω_i, GLQ weights; n, number of GLQ nodes; R_{ki}, remainder term; ε_2, maximum error in representation of right side of equation (1); ε, error of final result; x, spatial coordinate; $\varphi(t)$, $\psi(t)$, $u_0(x)$, known functions; W(x, t), heat flow function; K, number of subdivisions of interval of integration over the time.

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METHOD OF INVERSE DYNAMICAL SYSTEMS FOR THE RECONSTRUCTION OF INTERNAL SOURCES AND BOUNDARY CONDITIONS IN HEAT TRANSFER

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UDC 517.958+517.977

A method for the inversion of linear dynamical systems is described; it can be used to investigate several inverse problems in the reconstruction of boundary conditions or internal sources in linear transfer equations.

The inversion of a dynamical system (DS) involves the reconstruction of unknown input signals of the system from the results of measurements of the values of certain operators defined on the instantaneous states of the DS. In the theory of energy, momentum, and mass transfer the unknown signals can be both internal and external relative to the investigated effect: time-varying amplitudes of heat and mass sources and sinks; boundary transfer conditions, e.g., boundary temperatures, boundary heat inputs, time-varying contact resistances, etc. Instrumental inverse problems, whose objective is the reconstruction of a true signal from instrument readings [1], also belongs to the class of problems of reconstruction of DS inputs.

In the linear approximation an abstract mathematical model for a broad class of transfer processes exists in the form of a differential-operator system of equations

$$\frac{\partial w}{\partial t} = Lw + Bu(t), \quad w(0) = w_0, \tag{1}$$

$$lw = 0, \tag{2}$$

which is specified in a Hilbert space H. The element w_0 of H is the initial state of the process; $w:[0, \infty] \to H$ is the transfer potential; $Bu(\cdot)$ is the source function; l is a linear operator characterizing the boundary conditions; $B:U \to H$ and $L:H \to H$ are linear operators; U is the space of values of the function $u(\cdot)$. The specific choice of the operators L, l and the space H depends on the specific details of the transfer potential, e.g., whether it is in the form of a temperature field or an electromagnetic field, and also on the characteristics of the medium, the geometry of the system, and the boundary conditions. A natural constraint identifying the given class of systems of the form (1), (2) is the fact that the restriction A of the operator L onto the set of solutions of the equation $lw = 0$ is the generating operator of a semigroup e^{At}, which is strongly continuous at zero [2] (or, in other terminology,

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Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 55, No. 2, pp. 304-311, August, 1988. Original article submitted March 17, 1987.

0022-0841/88/5502-0934$12.50