NUMERICAL METHOD OF SOLVING CERTAIN NONLINEAR BOUNDARY-VALUE PROBLEMS IN HEAT AND MASS TRANSFER

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The gist of a numerical method of solving certain nonlinear boundary-value problems in heat- and mass-transfer theory is illustrated on an example of a one-dimensional such problem.

The numerical method which will be shown here is convenient for effectively solving certain boundary-value problems in heat- and mass-transfer theory, namely problems reducible to a system of nonlinear differential equations of the elliptic kind. Such problems arise, for instance, in the analysis of steady plain or magnetohydrodynamic flow of liquids through pipes and channels with variable transfer coefficients. When the transfer coefficients under laminar flow conditions are temperature-dependent, for example, then the dynamic problem and the thermal problem are tied together and a boundary-value problem involving a system of nonlinear equations can generally be solved by numerical methods only.

The gist of the proposed method can be explained on a simple example of a one-dimensional boundary-value problem which is described by a system of two ordinary differential equations:

$$\frac{d}{dx}\left(A\frac{du}{dx}\right)+F=0,\quad \frac{d}{dx}\left(B\frac{dv}{dx}\right)+G=0, \tag{1}$$

where the real positive coefficients A and B may arbitrarily depend on x, u, and v, while F and G can depend also on the derivatives u' and v'. On the interval $x_L \le x \le x_R$ we seek the solution to system (1) constrained by certain boundary conditions at points x_L and x_R. We will solve this problem by the stabilization method. System (1) is replaced by a system of parabolic partial differential equations:

$$\frac{\partial}{\partial x}\left(A\frac{\partial u}{\partial x}\right)+F=m_1^{-1}\frac{\partial u}{\partial t},\quad \frac{\partial}{\partial x}\left(B\frac{\partial v}{\partial x}\right)+G=m_2^{-1}\frac{\partial v}{\partial t}, \tag{2}$$

whose solution within the region $[x_L, x_R] \times [t_0, \infty]$ must satisfy the same boundary conditions and certain initial conditions. If there exists a solution to system (1) describing the stabilized process, then functions u(x, t) and v(x, t) after a sufficiently long time become steady and represent the sought solution to (1). In order to solve system (2) by the method of finite differences, we introduce a space grid and a time grid both generally nonuniform:

$$\begin{gathered} x_L = x_0 < x_1 < \ldots < x_i < \ldots < x_n = x_R,\quad \Delta x_i = x_{i+1} - x_i, \\ 0 = t_0 < t_1 < \ldots < t_k < \ldots,\quad \Delta t_k = t_{k+1} - t_k, \end{gathered} \tag{3}$$

and on them we construct an implicit difference scheme by the Tikhonov–Samarskii integrointerpolation method [1].

We will establish the difference analog of the first equation in (2). Letting

$$\xi_i = \frac{x_i + x_{i+1}}{2},\quad \varphi_i^k = \frac{1}{\Delta x_i}\int\limits_{x_i}^{x_{i+1}} u(x,\ t_k)\,dx,$$

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$$F_i^k = \frac{1}{\Delta x_i \Delta t_k} \int_{x_i}^{x_{i+1}} \int_{t_k}^{t_{k+1}} F(x,\ u(x,\ t),\ \ldots)\, dxdt,\quad i = 0 \text{ to } n-1,$$

$$p_i(t) = \left[\frac{\partial u}{\partial x}\right]_{x=x_i},\quad p_i^k = p_i(t_k),\quad i = 0 \text{ to } n,\quad k = 0,\ 1,\ 2,\ \ldots, \tag{4}$$

we integrate the first equation of system (2) over the region $[x_i, x_{i+1}] \times [t_k, t_{k+1}]$:

$$(\varphi_i^{k+1} - \varphi_i^k)\frac{\Delta x_i}{m_1} = \int_{t_k}^{t_{k+1}} \left([A]_{x=x_{i+1}} p_{i+1}(t) - [A]_{x=x_i} p_i(t)\right) dt + F_i^k \Delta x_i \Delta t_k, \tag{5}$$

$$i = 0 \text{ to } n-1,\quad k = 0,\ 1,\ 2,\ \ldots$$

According to [1], the integral is then replaced by its approximation:

$$\frac{1}{\Delta t_k} \int_{t_k}^{t_{k+1}} f(t)\, dt \approx \lambda f(t_{k+1}) + (1-\lambda) f(t_k). \tag{6}$$

In order to ensure the stability of the difference equations, it is sufficient to select $\lambda > 1/2$ ($\lambda = 1$ is a convenient choice, as it reduces the amount of computations).

The values p_i of space derivatives at the grid nodes x_i can be related to the average values φ_i of function u, if we integrate the approximate equality

$$u(x) \approx u(x_i) + (x - x_i)\, p_i = [u(x_i) - x_i p_i] + p_i x \tag{7}$$

with respect to x from x_{i-1} to x_i and from x_i to x_{i+1}; the sought approximation of the derivative is

$$p_i = \frac{\varphi_i - \varphi_{i-1}}{\xi_i - \xi_{i-1}},\quad i = 1 \text{ to } n-1. \tag{8}$$

Further considering only boundary conditions of the kind $u(x_L, t) = u_L$ and $u(x_R, t) = u_R$ for the derivatives at the boundary points, we obtain

$$p_0 = \frac{\varphi_0 - u_L}{\xi_0 - x_L},\quad p_n = \frac{u_R - \varphi_{n-1}}{x_R - \xi_{n-1}}. \tag{9}$$

With a fixed k, expression (5) with (6), (8), and (9) yields the sought system of difference equations

$$\begin{gathered} P_1 z_1 - (P_1 + P_0 + Q_0)\, z_0 = -R_0, \\ P_{i+1} z_{i+1} - (P_{i+1} + P_i + Q_i)\, z_i + P_i z_{i-1} = -R_i,\quad i = 1 \text{ to } n-2, \\ -(P_n + P_{n-1} + Q_{n-1})\, z_{n-1} + P_{n-1} z_{n-2} = -R_{n-1}, \end{gathered} \tag{10}$$

where $z_i = \varphi_i^{k+1}$ ($i = 0, \ldots, n-1$) and the coefficients are calculated according to the formulas

$$\begin{gathered} P_0 = \frac{A_0^{k+1}}{\xi_0 - x_L};\quad P_i = \frac{A_i^{k+1}}{\xi_i - \xi_{i-1}},\ i = 1 \text{ to } n-1;\ P_n = \frac{A_n^{k+1}}{x_R - \xi_{n-1}}; \\ Q_i = \frac{\Delta x_i}{m_1 \Delta t_k},\quad i = 0 \text{ to } n-1; \\ R_0 = P_0 u_L + Q_0(\varphi_0^k + m_1 \Delta t_k F_0^k); \\ R_i = Q_i(\varphi_i^k + m_1 \Delta t_k F_i^k),\quad i = 1 \div n-2; \\ R_{n-1} = P_n u_R + Q_{n-1}(\varphi_{n-1}^k + m_1 \Delta t_k F_{n-1}^k). \end{gathered} \tag{11}$$

In order to remove the nonlinearity, we replace t_{k+1} by t_k in the expression

$$A_i^{k+1} \equiv A\left(x_i,\ u(x_i,\ t_{k+1}),\ v(x_i,\ t_{k+1})\right)$$

and let

$$u(x_i, t_k) \approx \varphi_{i-1}^k + \frac{x_i - \xi_{i-1}}{\xi_i - \xi_{i-1}} (\varphi_i^k - \varphi_{i-1}^k), \quad i = 1 \text{ to } n-1 \tag{12}$$

with the same for $v(x_i, t_k)$. The quantities F_i^k, i.e., the values of function $F(x,u, v, u_x, v_x)$ averaged over the region $[x_i, x_{i+1}] \times [t_k, t_{k+1}]$ will be replaced by the values of F at $x = \xi_i$, $u = \varphi_i^k$, and $v = \psi_i^k$,

$$u_x = \begin{cases} \dfrac{\varphi_1^k - \varphi_0^k}{\xi_1 - \xi_0} \cdot \dfrac{\xi_0 - x_L}{\xi_1 - x_L} + \dfrac{\varphi_0^k - u_L}{\xi_0 - x_L} \cdot \dfrac{\xi_1 - \xi_0}{\xi_1 - x_L} & \text{at } i = 0, \\ \dfrac{\varphi_{i+1}^k - \varphi_i^k}{\xi_{i+1} - \xi_i} \cdot \dfrac{\xi_i - \xi_{i-1}}{\xi_{i+1} - \xi_{i-1}} + \dfrac{\varphi_i^k - \varphi_{i-1}^k}{\xi_i - \xi_{i-1}} \cdot \dfrac{\xi_{i+1} - \xi_i}{\xi_{i+1} - \xi_{i-1}} & \text{at } i = 1 \div n-2, \\ \dfrac{u_R - \varphi_{n-1}^k}{x_R - \xi_{n-1}} \cdot \dfrac{\xi_{n-1} - \xi_{n-2}}{x_R - \xi_{n-2}} + \dfrac{\varphi_{n-1}^k - \varphi_{n-2}^k}{\xi_{n-1} - \xi_{n-2}} \cdot \dfrac{x_R - \xi_{n-1}}{x_R - \xi_{n-2}} & \text{at } i = n-1 \end{cases} \tag{13}$$

and the same for v_x.

The difference analog of the second equation in (2) we establish by the same procedure; it has the form (10) for $z_i = \psi_i^{k+1}$ with appropriate obvious modifications in formulas (11)-(13).

Thus, the sought functions u and v have been approximated by their average values φ_i^k and ψ_i^k (at time $t = t_k$) over the intervals Δx_i. If φ_i^k and ψ_i^k are already determined, then the values of φ_i^{k+1} and ψ_i^{k+1} are found from the difference equations (10) solvable by the elimination method [2]. The elimination coefficients are calculated as follows:

$$V_{i+1} = \frac{P_{i+1}}{P_{i+1} + P_i(1 - V_i) + Q_i}, \quad W_{i+1} = \frac{P_i W_i + R_i}{P_{i+1} + P_i(1 - V_i) + Q_i}, \quad i = 0 \div n-1, \tag{14}$$

where $V_0 = W_0 = 0$, and then the solution

$$z_i = V_{i+1} z_{i+1} + W_{i+1}, \quad i = n-1, \ n-2, \ldots, 1, 0, \text{ where } z_n = 0. \tag{15}$$

is found.

The stabilization method may be regarded as an iteration method. The iteration is convergent with sufficiently small Δt steps, but a too small step will involve an unjustified longer computation time. On the other hand, the magnitude of the Δx steps has little effect on the convergence of the iterations. In setting up the algorithm on a computer, therefore, it is convenient to consider two stages. First, with a space grid, one selects the time scale factors m_1 and m_2 which will ensure convergence and a fast stabilization (without loss of generality, one may let $\Delta t = 1$). The following rule is useful for selecting m_1 and m_2:

$$m_1^{-1} \gtrsim \max_{x_i} \left| \frac{\partial F}{\partial u} \right|, \quad m_2^{-1} \gtrsim \max_{x_i} \left| \frac{\partial G}{\partial v} \right|. \tag{16}$$

Then in order to obtain the required accuracy of the solution, one switches to a denser space grid.

It is quite evident that the implicit scheme (10)-(11), as an analog of system (2), represents a first-order approximation. With an increasing number of nodes n in the space grid, therefore, the error decreases rather slowly (as n^{-1}). The accuracy of the solution can be improved significantly by utilizing the feasibility of a nonuniform x_i-grid with the specific character of the sought solution properly taken into consideration.

One absolute advantage of this stabilization method is the feasibility of checking both the existence and the stability of the solution while the latter is constructed.

The procedure shown here can, without difficulty, be extended to two-dimensional problems (e.g., in using the method of variable directions [3] with respect to orthogonal coordinate axes).

An application of this method in the problem of fluid flow with variable transfer coefficients through an MHD channel [4] has demonstrated its great advantages over other earlier methods used for solving this problem [5]. For instance, this method is much more economical and accurate than the known method of coupled equations [6]; another important feature of this method is its effectiveness in solving the problem when the coefficients of the lower-order derivatives are small. Thus, it has been possible to obtain very accurate solutions to the said problem in [4], with the Hartmann number and the nonisothermality factor by a few orders of magnitude higher than would have been possible by the method of coupled equations.

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