

ON THE QUESTION OF NUMERICAL INTEGRATION OF PARABOLIC EQUATIONS

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Abstract

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MATHEMATICS

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ON THE QUESTION OF NUMERICAL INTEGRATION OF PARABOLIC EQUATIONS

(Presented by Academician A. A. Dorodnitsyn, 23 V 1957)

All known difference methods for the numerical integration of parabolic and hyperbolic equations of mathematical physics can be divided into two groups, depending on whether or not, for the computation of the next step, they require the solution of a system of algebraic equations. Methods belonging to the first group ("explicit") are simple, but for stability of the computation they impose a severe restriction on the steps. Methods of the second group ("implicit"), on the contrary, are more complicated, but are stable for arbitrary ratios of the steps.

In our note ⁽¹⁾ an explicit method with a weaker stability restriction was considered. However, in comparison with the above-mentioned classical methods of both groups, this method has a greater error, namely $C_{\Delta x}\Delta x + O((\Delta x)^2)$, where $C_{\Delta x}$ tends to zero more slowly than Δx , instead of $O((\Delta x)^2)$ in the cases mentioned above.

In the present paper another explicit method is considered, which has error $O((\Delta x)^2)$ and has a weaker stability restriction. In addition, one explicit method is considered which is convenient for use on high-speed computing machines.

For simplicity, all further reasoning will be carried out for the simplest problem

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial u}{\partial t}, \quad 0 < x < 1, \quad t > 0; \quad u(x, 0) = f(x); \quad u(0, t) = u(1, t) = 0. \quad (1)$$

Let Δx and Δt denote the steps, respectively, in x and t . Put

$$\begin{aligned}
 S^{(m)}u_{0,k}^{(i)} = & \frac{\alpha^m}{2(\omega + \alpha)^m} (u_{-m,k+1} + u_{m,k+1}) + \\
 & + \frac{\alpha^{m-1}(1 - \alpha)}{2(\omega + \alpha)^m} (u_{-m,k} + u_{m,k}) + \frac{\alpha^{m-2}(\omega - \alpha)}{2(\omega + \alpha)^m} (u_{m-1,k} + u_{-(m-1),k}) + \\
 & + \frac{\omega^2}{2(\omega + \alpha)^2} \sum_{\gamma=1}^{m-2} \frac{\alpha^{\gamma-1}}{(\omega + \alpha)^\gamma} (u_{-\gamma,k} + u_{\gamma,k}) + \\
 & + \frac{\delta\alpha + (\omega + \alpha)^2 - 2(\omega + \alpha)}{(\omega + \alpha)^2} u_{0,k} + \frac{1}{2(\omega + \alpha)} (u_{-1,k} + u_{1,k}) \quad (m = 1, 2, \dots),
 \end{aligned}$$

where $u_{\pm p,q}^{(i)} = u((i \pm p)\Delta x, q\Delta t)$ (the upper index (i) , if this causes no misunderstanding, is omitted); $\omega = (\Delta x)^2/\Delta t = \text{const} > 0$; $\delta = 0$ for $m = 1$ and $\delta = 1$ for $m > 1$; $0 \leq \alpha \leq 1$. We write the functional equation

$$u_{0,k+1}^{(i)} = S^{(m)}u_{0,k}^{(i)}. \tag{2}$$

In particular, for $m = \alpha = 1$, equation (2) gives the implicit method described by Crank and Nicolson ⁽²⁾ (schematically * * *),

$$u_{0,k+1}^{(i)} = S^{(1)}u_{0,k}^{(i)} = \frac{1}{2(1 + \omega)} [u_{-1,k+1} + u_{1,k+1} + u_{1,k} + u_{-1,k} + 2(1 - \omega)u_{0,k}].$$

For $m = 2$, $\alpha = 1$, we obtain another implicit difference scheme

$$u_{0,k+1}^{(i)} = S^{(2)}u_{0,k}^{(i)} = \frac{1}{2(1 + \omega)^2} [u_{-2,k+1} + u_{2,k+1} + 2\omega(u_{1,k} + u_{-1,k} + \omega u_{0,k})]$$

(schematically * * *).

Formula (2) also provides an explicit algorithm for the numerical integration of problem (1). Let, for example, $\Delta x = 1/2^N$. Then the explicit computation of the $(k + 1)$ -st layer ($t = (k + 1)\Delta t$) from the k -th layer ($t = k\Delta t$) and the boundary conditions can be carried out as follows:

$$\begin{aligned}
 u_{0,k+1}^{(2^{N-1})} = & S^{(2^{N-1})}u_{0,k}, \\
 u_{0,k+1}^{(2^{N-2})} = & S^{(2^{N-2})}u_{0,k}, \quad u_{0,k+1}^{(3 \cdot 2^{N-2})} = S^{(2^{N-2})}u_{0,k}, \\
 & \dots \dots \dots \tag{3}
 \end{aligned}$$

$$u_{0,k+1}^{(1)} = S^{(1)}u_{0,k}, \quad u_{0,k+1}^{(3)} = S^{(1)}u_{0,k}, \dots, u_{0,k+1}^{(2^N-1)} = S^{(1)}u_{0,k}.$$

Here the operators $S^{(2^N-j)}$ are used 2^{j-1} times ($j = 1, 2, \dots, N$). In particular, for $\Delta x = 1/8$, $\omega = \alpha = 1$, formulas of the following types must be applied

$$u_{0,k+1}^{(i)} = \frac{1}{32} [u_{-4,k+1} + u_{4,k+1} + u_{-2,k} + u_{2,k} + 10(u_{-1,k} + u_{1,k}) + 8u_{0,k}] \quad (i = 4);$$

$$u_{0,k+1}^{(i)} = \frac{1}{8} [u_{-2,k+1} + u_{2,k+1} + 2(u_{-1,k} + u_{0,k} + u_{1,k})] \quad (i = 2, 6);$$

$$u_{0,k+1}^{(i)} = \frac{1}{4} (u_{-1,k+1} + u_{1,k+1} + u_{-1,k} + u_{1,k}) \quad (i = 1, 3, 5, 7)$$

1, 2, and 4 times, respectively.

Applying the corresponding Taylor-series expansions, one can show that difference equation (2) (or (3)) approximates the differential equation of problem (1) with an error $O((\Delta x)^2)$. Here the coefficient of $(\Delta x)^2$ is proportional, for example in the case $\omega = \alpha = 1$, to the quantity $13/12 - m/(2^m - 1)$, whence, in particular, it follows that the smallest error occurs for $m = 1$ (the Crank-Nicolson case).

When solving on high-speed computing machines, method (3) is inconvenient because of the nonuniformity of the formulas.

We point out the following modification of it, free of the indicated drawback. Each step in t is computed twice: from left to right by the formulas

$$u_{i,k+1} = \frac{1}{\omega + \alpha} [\alpha u_{i-1,k+1} + (1 - \alpha)u_{i-1,k} + u_{i+1,k} - (2 - \omega - \alpha)u_{i,k}], \quad (4)$$

and from right to left by the formulas

$$u_{i,k+1} = \frac{1}{\omega + \alpha} [\alpha u_{i+1,k+1} + (1 - \alpha)u_{i+1,k} + u_{i-1,k} - (2 - \omega - \alpha)u_{i,k}]. \quad (5)$$

The arithmetic mean of these two computations gives the desired result (here the usual notation $u_{i,k} = u(i\Delta x, k\Delta t)$ has been used). In what follows we shall call this method the method (4)–(5).

In matrix form equation (4) can be written as follows:

$$u^{(k+1)} = Au^{(k)}, \quad (6)$$

where

$$u^{(k)} = \{u_{1,k}, u_{2,k}, \dots, u_{n,k}\}, \quad n = \frac{1}{\Delta x} - 1;$$

$$A = \frac{1}{\omega + \alpha} \times \begin{pmatrix} \omega - \alpha - 2 & 1 & & & \\ \left(1 - \frac{2\alpha}{\omega + \alpha}\right) & C & 1 & & \\ \frac{\alpha}{\omega + \alpha} \left(1 - \frac{2\alpha}{\omega + \alpha}\right) & \frac{\omega^2}{(\omega + \alpha)^2} & C & & \\ \dots & \dots & \dots & \dots & \dots \\ \left(\frac{\alpha}{\omega + \alpha}\right)^{n-2} \left(1 - \frac{2\alpha}{\omega + \alpha}\right) & \frac{\alpha^{n-3}\omega^2}{(\omega + \alpha)^{n-1}} & \frac{\alpha^{n-4}\omega^2}{(\omega + \alpha)^{n-2}} & \dots & C \end{pmatrix},$$

$$C = \frac{\omega^2 - (2\omega + \alpha)(1 - \alpha)}{\omega + \alpha}.$$

Estimating the absolute value of the largest eigenvalue of the matrix A by its norm (by rows), we obtain the following sufficient stability condition (uniformly in n):

$$\Delta t \leq \frac{(\Delta x)^2}{\max\{3/2 - \alpha; 1 - \alpha + \sqrt{1 - \alpha}\}}. \quad (7)$$

In particular, for $\alpha = 0$, inequality (7) becomes the well-known stability condition $\Delta t \leq (\Delta x)^2/2$ (in this case equation (6) becomes the corresponding classical difference equation).

Next, if the influence of numerical errors at the boundary and near-boundary nodes (x_0, t_k) , (x_1, t_k) , (x_2, t_k) and (x_{n+1}, t_k) , (x_n, t_k) , (x_{n-1}, t_k) ($k = 1, 2, \dots$) is neglected, then it can be shown that method (4)–(5) is stable if the condition

$$\Delta t \leq \frac{(\Delta x)^2}{2(1 - \alpha)} \quad (8)$$

is satisfied.

For comparison of the different methods we give Table 1.

Table 1

	Classical methods (methods 1) and 2) according to the terminology of ⁽¹⁾ explicit $\Delta t = (\Delta x)^2/2$	Classical methods (methods 1) and 2) according to the terminology of ⁽¹⁾ explicit $\Delta t = (\Delta x)^2$	Classical methods (methods 1) and 2) according to the terminology of ⁽¹⁾ implicit $\Delta t = (\Delta x)^2$	Method (3), $\alpha =$	Method (4)–(5), $\alpha =$	Exact values
0	0	0	0	0	0	0
Δx	0,1530	0,6875	0,1690	0,1653	0,1626	0,1564
$2\Delta x$	0,2817	−0,5000	0,3120	0,3068	0,3094	0,2892
$3\Delta x$	0,3692	1,0625	0,4073	0,4011	0,4094	0,3779
$4\Delta x$	0,3984	−0,2500	0,4407	0,4378	0,4449	0,4091

Here $f(x) = 4x(1 - x)$, $\Delta x = 1/8$ (by virtue of the symmetry of the initial function $f(x)$, only half the values are given), $t = 6(\Delta x)^2$. It follows from the table that, for $\Delta t = (\Delta x)^2$, the explicit classical method gave an absurd result (failure of the stability condition). The other three methods (for the same value of Δt) gave approximately the same error.

Table 2

	Method (3), $\omega = 1, \alpha = 1/2$	Method (4)–(5), $\omega = 1, \alpha = 1/2$	Exact values
0	0	0	0
Δx	0.1557	0.1550	0.1564
$2\Delta x$	0.2850	0.2860	0.2892
$3\Delta x$	0.3752	0.3780	0.3779
$4\Delta x$	0.4045	0.4067	0.4091

With a decrease of the weight α of the “part” of the second “derivative” with respect to x on the unknown layer, the stability condition, generally speaking, as follows from (7) and (8), becomes more stringent. At the same time, with decreasing α , the accuracy of methods (3) and (4)–(5) increases noticeably; for example, for equation (4) the error has the form $O(\alpha\Delta x)$. Thus, for $\alpha = 1/2$, methods (3) and (4)–(5), under the same conditions as above, give the results presented in Table 2.

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CITED LITERATURE

1. V. K. Saul' yev, DAN, **115**, No. 6 (1957).

2. J. Crank, P. Nicolson, Proc. Cambridge Phil. Soc., **43**, 50 (1947).

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