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Time Step Selection for the Numerical Solution of Boundary Value Problems for Parabolic Equations

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Abstract—An algorithm is proposed for selecting a time step for the numerical solution of boundary value problems for parabolic equations. The solution is found by applying unconditionally stable implicit schemes, while the time step is selected using the solution produced by an explicit scheme. Explicit computational formulas are based on truncation error estimation at a new time level. Numerical results for a model parabolic boundary value problem are presented, which demonstrate the performance of the time step selection algorithm.

Keywords: implicit difference schemes, time step selection, parabolic equation, truncation error.

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INTRODUCTION

Primary attention in the approximate solution of boundary value problems for time-dependent equations is given to time approximations [1–3]. For second-order parabolic equations, unconditionally stable schemes are constructed using implicit approximations [4–6]. Two-level schemes are the most popular in numerical practice, while schemes with three and more time levels are used much less frequently. For unconditionally stable schemes, the choice of a time step is determined only by the accuracy of the approximate solution.

The problem of time step control has been relatively well studied in the case of the Cauchy problem for systems of differential equations [7–9]. The basic approach is that the error of the approximate solution is estimated at a new time level via additional computations, the time step is estimated using the theoretical asymptotic dependence of accuracy on the time step, and, if necessary, the time step is corrected and the computations are repeated.

Additional computations for estimating the error of the approximate solution can be based on different approaches. Specifically, an approximate solution can be obtained using two different schemes of the same theoretical order of accuracy. The best known example of this strategy is the solution of a problem at a certain time interval with the use of a given time step (first solution) and a halved time step (second solution). The approximate solution of Cauchy problems for systems of ordinary differential equations can also be based on nested methods. In this case, two approximate solutions with different orders of accuracy are compared.

In fact, the indicated techniques for time step selection belong to the class of a posteriori error estimation methods. In this case, whether the time step is suitable or has to be changed (increased or decreased and how much) and whether repeated computations are needed is decided after the solution has been computed. Similar strategies can also be used on the basis of a more advanced a posteriori analysis of approximate solutions of time-dependent boundary value problems (see [10–12]).

In fact, a priori time step selection for the approximate solution of boundary value problems for parabolic equations was considered in [13]. Some more general problems were addressed in [14]. The solution at a new time level was found by applying the standard implicit Euler scheme. The time step at the new level was explicitly calculated using the solutions from two previous time levels with variations in the coefficients of the equation and in the right-hand side taken into account.

In this paper, we explore new possibilities of time step estimation for the approximate solution of boundary value problems for parabolic equations based on an auxiliary solution produced by an explicit scheme. In [13, 14] the time step was estimated by comparing numerical solutions, namely, using an error estimate for the approximate solution. In this work, we use a more direct approach based on truncation error estimation.

1. FORMULATION OF THE PROBLEM

We consider the Cauchy problem for the linear equation

$$\frac{du}{dt} + A(t)u = f(t), \quad 0 < t \le T, \tag{1.1}$$

with the initial condition

$$u(0) = u_0. \tag{1.2}$$

The problem is studied in a finite-dimensional Hilbert space H. Assume that

$$A(t) \ge 0$$

in H. Since the operator A of problem (1.1), (1.2) is nonnegative, its solution satisfies the following estimate of stability with respect to the initial data and the right-hand side:

$$\|u(t)\| \le \|u_0\| + \int_0^t \|f(\theta)\| d\theta. \tag{1.3}$$

Problem (1.1), (1.2) arises when a finite difference, finite volume, or finite element approximation (lumped mass scheme [15]) is applied to boundary value problems for a second-order parabolic equation. In this problem, the unknown function $u(x,t)$ satisfies the equation

$$\frac{\partial u}{\partial t} - \sum_{\alpha=1}^{m} \frac{\partial}{\partial x_\alpha}\left(k(\mathbf{x},t)\frac{\partial u}{\partial x_\alpha}\right) + p(\mathbf{x},t)u = f(\mathbf{x},t), \quad \mathbf{x} \in \Omega, \quad 0 < t \le T,$$

where $\underline{k} \le k(\mathbf{x},t) \le \overline{k}$, $\mathbf{x} \in \Omega$, $\underline{k} > 0$, and $p(\mathbf{x},t) \ge 0$. The equation is supplemented with the Dirichlet boundary conditions

$$u(\mathbf{x},t) = g(\mathbf{x},t), \quad \mathbf{x} \in \partial\Omega, \quad 0 < t \le T$$

and the initial condition

$$u(\mathbf{x},0) = u_0(\mathbf{x}), \quad \mathbf{x} \in \Omega.$$

This time-dependent problem is solved numerically on a nonuniform grid in time:

$$t_0 = 0, \quad t_{n+1} = t_n + \tau_{n+1}, \quad n = 0,1,\ldots,N-1, \quad t_N = T.$$

Let $f_n = f(t_n)$. For problem (1.1), (1.2), we use a fully implicit scheme whereby the transition from one time level to another is given by the equality

$$\frac{y_{n+1} - y_n}{\tau_{n+1}} + A_{n+1}y_{n+1} = f_{n+1}, \quad n = 0,1,\ldots,N-1, \tag{1.4}$$

and the initial condition

$$y_0 = u_0. \tag{1.5}$$

Under the restriction $A_{n+1} \ge 0$, it follows directly from (1.4) that the approximate solution satisfies the levelwise estimate

$$\|y_{n+1}\| \le \|y_n\| + \tau_{n+1}\|f_{n+1}\|.$$

Thus, we obtain a discrete analogue of estimate (1.3) for problem (1.4), (1.5), namely,

$$\|y_{n+1}\| \le \|u_0\| + \sum_{k=0}^{n} \tau_{k+1}\|f_{k+1}\|. \tag{1.6}$$

The error of the approximate solution $z_n = y_n - u_n$ satisfies the problem

$$\frac{z_{n+1} - z_n}{\tau_{n+1}} + A_{n+1} z_{n+1} = \psi_{n+1}, \quad n = 0, 1, \ldots, N-1,$$

$$z_0 = 0.$$

Here, ψ_{n+1} is the truncation error:

$$\psi_{n+1} = f_{n+1} - \frac{u_{n+1} - u_n}{\tau_{n+1}} - A_{n+1} u_{n+1}. \tag{1.7}$$

In a similar manner to (1.6), we have the following estimate for the error:

$$\|z_{n+1}\| \le \sum_{k=0}^{n} \tau_{k+1} \|\psi_{k+1}\|. \tag{1.8}$$

Accordingly, for error control, we can use the summarized error $\tau_{n+1}\delta$ over the interval $t_n \le t \le t_{n+1}$. In this case, the number δ determines the same level of error over the entire integration interval. It follows from (1.8) that the error of the approximate solution satisfies the estimate

$$\|z_{n+1}\| \le \delta t_{n+1}.$$

The error accumulates and grows linearly with time.

The basic feature of our approach is that a numerical solution of the time-dependent problem is found by applying an unconditionally stable implicit scheme. This scheme makes the basic contribution to the computational costs required for the transition to a new time level. An explicit scheme is far less costly and conditionally stable, but it is unstable for the time steps used. In fact, it is used only to estimate the discrepancy of the implicit scheme. Therefore, our algorithm is stable, and its stability is completely determined by the properties of the basic implicit scheme.

2. ALGORITHM FOR TIME STEP ESTIMATION

By virtue of error estimate (1.8) for the approximate solution, the accumulation of errors in the transition from the time level t_n to the next one t_{n+1} is governed by to the rule

$$\|z_{n+1}\| \le \|z_n\| + \tau_{n+1} \|\psi_{n+1}\|.$$

Accordingly, we need to monitor the local error ψ_{n+1}.

If we could calculate the truncation error ψ_{n+1}, we would obtain an a posteriori error estimate. Comparing $\|\psi_{n+1}\|$ with the prescribed error level δ, we could evaluate the quality of the chosen time step τ_{n+1}. Namely, if $\|\psi_{n+1}\|$ is much larger (smaller) than δ, then the time step is too large (small), and if $\|\psi_{n+1}\|$ is close to δ, then the time step is optimal. Thus,

$$\tau_{n+1}: \|\psi_{n+1}\| \approx \delta. \tag{2.1}$$

The difficulty is that we cannot calculate the truncation error, since it is determined using the exact solution, which is not known. Accordingly, we have to use estimates for the truncation error that guarantee the fulfillment of (2.1).

The general approach to adaptive time step selection in the approximate solution of time-dependent problems consists of the following basic elements:

- the selection of a prognostic time step by analyzing the solution obtained at the preceding time steps;
- computations with the prognostic time step;
- an analysis of the accuracy of the resulting approximate solution and, if necessary, recalculation with a smaller time step.

This general strategy is usually implemented (see, e.g., [7–9]) via an asymptotic analysis of the error of the approximate solution, provided that the error does not vary significantly with time. Let us note the basic distinctive features of our approach to time step selection.

In our case, the prognostic time step is fixed: we always want to increase the time step, relying on its current value. To estimate the time step at a new time level (in the transition from t_n to the next time t_{n+1}), we use the preceding time step $\tau_n = t_n - t_{n-1}$. The primary goal is to use a larger time step at the new time level. In this context, the prognostic time step is defined as

$$\tilde{\tau}_{n+1} = \gamma\tau_n, \tag{2.2}$$

where γ is a numerical parameter of the algorithm. For a maximum increase in the time step, γ is set equal, for example, to 1.25 or 1.5. The parameters of the problem (the coefficients and right-hand side of the equation and their variations) are estimated on the interval $[t_n, t_n + \tilde{\tau}_{n+1}]$. When estimating the time step, we need to determine the moment of time when the parameters of the problem change substantially.

Under the restriction $\tilde{\tau}_{n+1}$, the time step is chosen using computational formulas based on the estimate of the truncation error at a new time level. An approximate solution at the new time level is found by applying implicit scheme (1.4), while the time step is estimated using the explicit scheme. Both (explicit and implicit) schemes have the same order of accuracy, and the new approximate solution is computed using the same initial condition (at $t = t_n$). Since the computation is performed over only one time step, possible computational instability for the explicit scheme is not exhibited.

The following strategy is proposed for correcting the time step. The step τ_{n+1} is determined by the following conditions:

Prognostic solution. The explicit scheme is used to compute the solution $\tilde{y}_{n+1}$ at the time $\tilde{t}_{n+1} = t_n + \tilde{\tau}_{n+1}$.

Truncation error. The found $\tilde{y}_{n+1}$ and the implicit scheme are used to estimate the truncation error.

Step selection. The step τ_{n+1} is evaluated via the proximity of the error norm to δ (see condition (2.1)).

Let us present the computational formulas for time step selection. The prognostic solution $\tilde{y}_{n+1}$ is determined by the equation

$$\frac{\tilde{y}_{n+1} - y_n}{\tilde{\tau}_{n+1}} + A_n y_n = f_n. \tag{2.3}$$

Next, this solution is used to estimate the truncation error of the implicit scheme in the transition from the time t_n to $\tilde{t}_{n+1}$.

According to (1.7), the truncation error is calculated using the exact solution at two times, namely, at t_n and $\tilde{t}_{n+1}$. In the error estimation procedure, $u(t_n)$ and $u(\tilde{t}_{n+1})$ have to be somehow evaluated. Instead of $u(t_n)$, we use y_n. Thus, we estimate the truncation error over a single step, assuming that y_n is the exact initial data at the time level. The exact solution $u(\tilde{t}_{n+1})$ at the new level is replaced by the approximate solution $\tilde{y}_{n+1}$ produced by explicit scheme (2.3). Accordingly, we set

$$\tilde{\psi}_{n+1} = \tilde{f}_{n+1} - \frac{\tilde{y}_{n+1} - y_n}{\tilde{\tau}_{n+1}} - \tilde{A}_{n+1}\tilde{y}_{n+1}. \tag{2.4}$$

Here, we used the notation

$$\tilde{f}_{n+1} = f(t_n + \gamma\tau_n), \quad \tilde{A}_{n+1} = A(t_n + \gamma\tau_n).$$

The truncation error $\tilde{\psi}_{n+1}$ is identified with the time step $\tilde{\tau}_{n+1}$, and ψ_{n+1}, with the step τ_{n+1}. In view of (2.1), we set

$$\bar{\tau}_{n+1} = \gamma_{n+1}\tau_n, \quad \gamma_{n+1} = \frac{\delta}{\|\tilde{\psi}_{n+1}\|}\gamma. \tag{2.5}$$

The desired time step cannot exceed the prognostic one, so

$$\tau_{n+1} \le \bar{\tau}_{n+1}, \quad \tau_{n+1} \le \tilde{\tau}_{n+1}.$$

It is natural to restrict the admissible time step from below by a minimum step τ_0. In view of this, we set

$$\tau_{n+1} = \max\{\tau_0, \min\{\gamma_{n+1}, \gamma\}\tau_n\}. \tag{2.6}$$

According to (2.3)–(2.6), the computational formulas for time step selection can be specified as follows. Substituting (2.4) into (2.5) yields

$$\begin{aligned}\tilde{\psi}_{n+1} &= \tilde{f}_{n+1} - f_n - \tilde{A}_{n+1}\tilde{y}_{n+1} + A_n y_n = \tilde{f}_{n+1} - f_n \\ &\quad - (\tilde{A}_{n+1} - A_n)y_n - \tilde{A}_{n+1}(\tilde{y}_{n+1} - y_n) \\ &= \tilde{\tau}_{n+1}\left(\frac{\tilde{f}_{n+1} - f_n}{\tilde{\tau}_{n+1}} - \frac{\tilde{A}_{n+1} - A_n}{\tilde{\tau}_{n+1}} y_n - \tilde{A}_{n+1}\frac{\tilde{y}_{n+1} - y_n}{\tilde{\tau}_{n+1}}\right).\end{aligned}$$

Thus, the estimated truncation error is if the first order in time:

$$\tilde{\psi}_{n+1} = \mathbb{O}(\tilde{\tau}_{n+1}).$$

Accordingly, we set

$$\|\tilde{\psi}_{n+1}\| \le \|\tilde{f}_{n+1} - f_n - (\tilde{A}_{n+1} - A_n)y_n - \tilde{A}_{n+1}(\tilde{y}_{n+1} - y_n)\|. \tag{2.7}$$

Combining (2.7) with (2.5), we obtain formula (2.6) for calculating the time step, where

$$\gamma_{n+1} = \frac{\delta}{\|\tilde{f}_{n+1} - f_n - (\tilde{A}_{n+1} - A_n)y_n - \tilde{A}_{n+1}(\tilde{y}_{n+1} - y_n)\|}\gamma. \tag{2.8}$$

This formula (see the denominator in the expression for γ_{n+1}) reflects the corrections in the time step selection procedure that are related to the time dependence of the right-hand side (first part) and of the problem operator (second part) and to the time variation in the solution (third part).

Similar formulas for time step selection were obtained in [13, 14] by estimating the variation in the approximate solution obtained after two auxiliary steps with a prognostic time step. The first (forward) step was based on an explicit scheme, while the second step, on an explicit backward scheme. Here, we used a simpler and more general procedure for truncation error estimation at a prognostic time step, namely, the approximate solution produced after a single forward step of the explicit scheme was used.

3. GENERALIZATIONS

The approach proposed for time step selection can be used in many other problems. We describe the simplest possibilities associated with second-order accurate time schemes for the approximate solution of model problem (1.1), (1.2).

Problem (1.1), (1.2) can be solved numerically by applying the following symmetric (Crank–Nicolson) scheme rather than the fully implicit one (1.4):

$$\frac{y_{n+1} - y_n}{\tau_{n+1}} + \frac{A_{n+1} + A_n}{2}\frac{y_{n+1} + y_n}{2} = \frac{f_{n+1} + f_n}{2}, \quad n = 0, 1, \dots, N-1. \tag{3.1}$$

A potential advantage of this scheme is that it has a higher (second) order of accuracy in time than scheme (1.4), which is first-order accurate.

The time step in scheme (1.5), (3.1) is now estimated by applying a second-order accurate explicit scheme. Remaining in the class of two-level schemes, instead of (2.3), we use

$$\frac{\tilde{y}_{n+1} - y_n}{\tilde{\tau}_{n+1}} + A_n y_n - \frac{\tilde{\tau}_{n+1}}{2}A_n^2 y_n = \frac{\tilde{f}_{n+1} + f_n}{2} - \frac{\tilde{\tau}_{n+1}}{2}A_n f_n. \tag{3.2}$$

Other second-order accurate explicit Runge–Kutta schemes can be used instead of (3.2).

Another interesting possibility is associated with second-order accurate three-level schemes. Specifically, such a scheme on a nonuniform grid in time can be written as

$$\theta\frac{\tilde{y}_{n+1} - y_n}{\tilde{\tau}_{n+1}} + (1-\theta)\frac{y_n - y_{n-1}}{\tau_n} + A_n y_n = f_n, \quad n = 1, 2, \dots, N-1, \tag{3.3}$$

where y_0 and y_1 are given. The solution y_1 is calculated with a minimum step: $\tau_1 = \tau_0$. The weight parameter θ is given by

$$\theta = \frac{\gamma}{1+\gamma}.$$

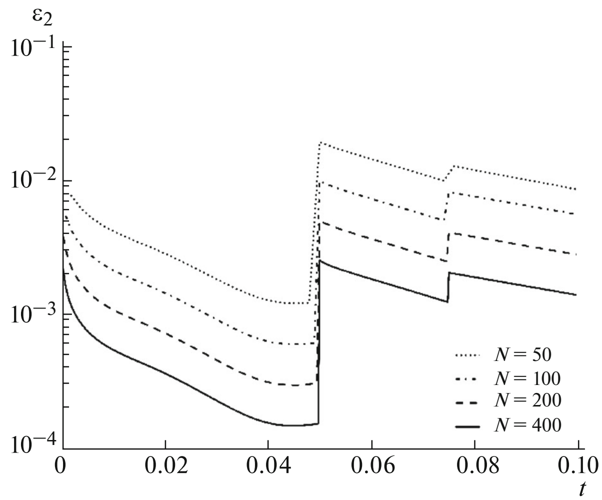

Fig. 1. Error in the $L_2(\omega)$ norm on a uniform grid.

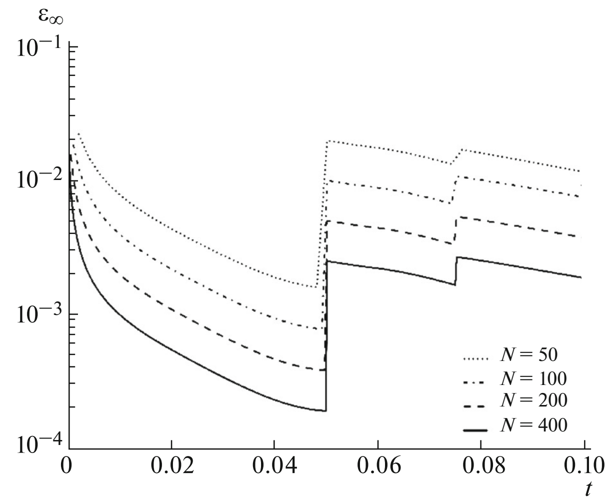

Fig. 2. Error in the $L_\infty(\omega)$ norm on a uniform grid.

In a similar manner to (2.4), for scheme (3.1), we set

$$\tilde{\psi}_{n+1} = \frac{\tilde{f}_{n+1} + f_n}{2} - \frac{\tilde{y}_{n+1} - y_n}{\tau_{n+1}} - \frac{\tilde{A}_{n+1} + A_n}{2} \frac{\tilde{y}_{n+1} + y_n}{2}, \tag{3.4}$$

where $\tilde{y}_{n+1}$ is found using scheme (3.2) or (3.3). The truncation error is

$$\tilde{\psi}_{n+1} = \mathbb{O}(\tilde{\tau}_{n+1}^2).$$

Assigning $\tilde{y}_{n+1}$ to $\tilde{\tau}_{n+1}^2$ and δ to the new time step τ_{n+1}^2, by analogy with (2.5), we obtain the expression

$$\bar{\tau}_{n+1} = \gamma_{n+1}\tau_n, \quad \gamma_{n+1} = \left(\frac{\delta}{\|\tilde{\psi}_{n+1}\| \,||}\right)^{1/2} \gamma \tag{3.5}$$

for estimating the time step.

The algorithm for time step selection remains the same as before: the solution at a prognostic time step is produced by the explicit scheme with the use of (3.2) or (3.3), the truncation error at this step is calculated using formula (3.4), and the time step is estimated according to (2.6) and (3.5). The solution at a new time level is found by applying scheme (3.1).

4. NUMERICAL EXPERIMENTS

To illustrate the performance of algorithm (2.5), (2.6) for time step selection in the case an implicit scheme used to solve problem (1.1), (1.2), we considered a boundary value problem for a one-dimensional parabolic equation. Suppose that $u(x,t)$ satisfies the equation

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} + p(t)u = f(t), \quad 0 < x < 1, \quad 0 < t \le T, \tag{4.1}$$

and obeys the boundary and initial conditions

$$u(0,t) = 0, \quad u(1,t) = 0, \quad 0 < t \le T, \tag{4.2}$$

$$u(x,0) = u_0(x), \quad 0 < x < 1. \tag{4.3}$$

Problem (4.1)–(4.3) was solved using a finite difference approximation in space. We introduced a uniform grid with a step h:

$$\bar{\omega} = \{x | x = ih,\ i = 0,1,\ \ldots,\ M,\ Mh = 1\},$$

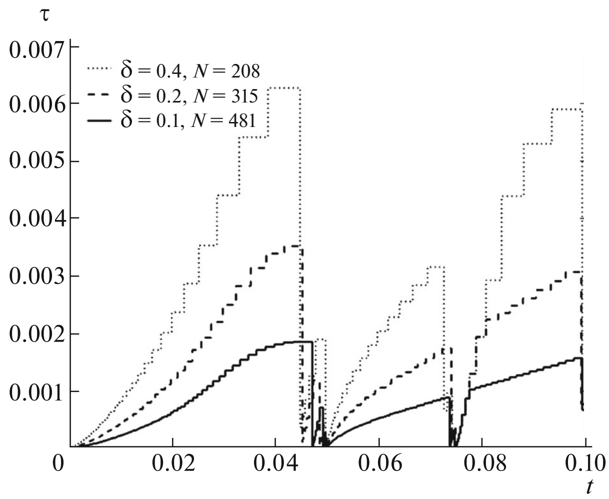

Fig. 3. Time steps, the $L_2(\omega)$ norm.

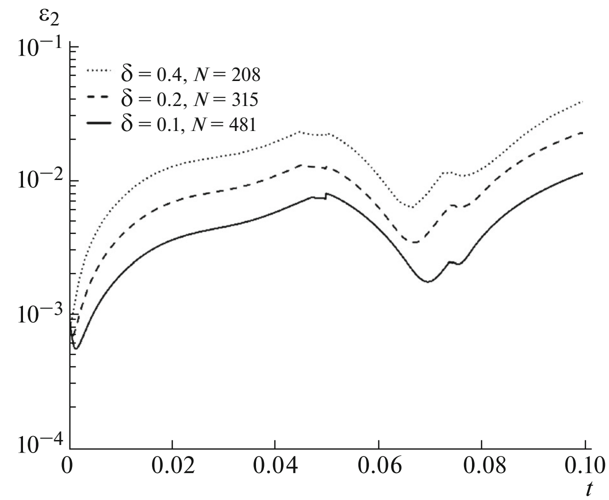

Fig. 4. Error in the $L_2(\omega)$ norm on a nonuniform grid.

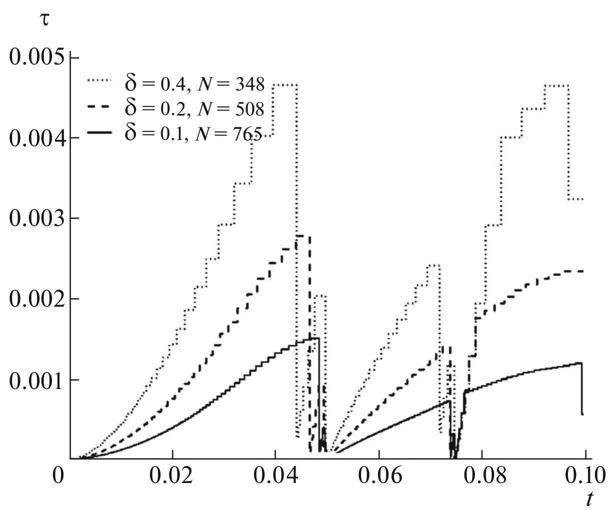

Fig. 5. Time steps, the $L_\infty(\omega)$ norm.

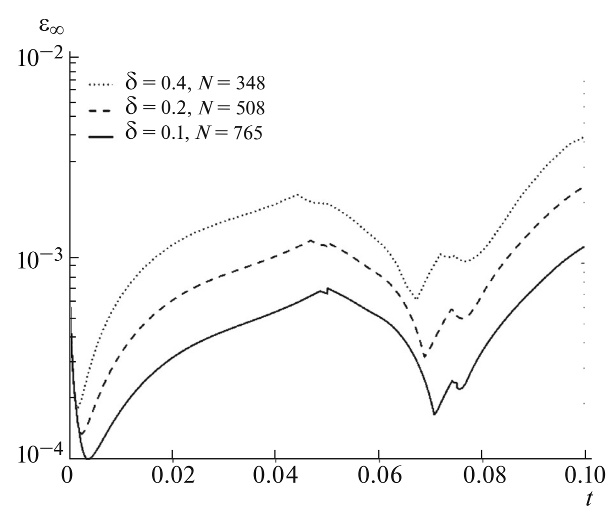

Fig. 6. Error in the $L_\infty(\omega)$ norm on a nonuniform grid.

where ω is the set of interior nodes and $\partial\omega$ is the set of boundary nodes ($\bar{\omega} = \omega \cup \partial\omega$). On the set of grid functions such that $u(x) = 0$, $x \notin \omega$, we defined a Hilbert space H with the inner product and norm given by

$$(u, v) = \sum_{x \in \omega} u(x)v(x)dx, \qquad \|u\| = (u, u)^{1/2}.$$

The grid operator $A(t)$ was specified as

$$Au = -\frac{1}{h^2}(u(x+h) - 2u(x) + u(x-h)) + p(t)u(x), \qquad x \in \omega.$$

The operator $A(t)$ is self-adjoint and, for $p(t) \geq 0$, it is positive definite in H. Thus, the spatial discretization of (4.1)–(4.3) yields problem (1.1), (1.2).

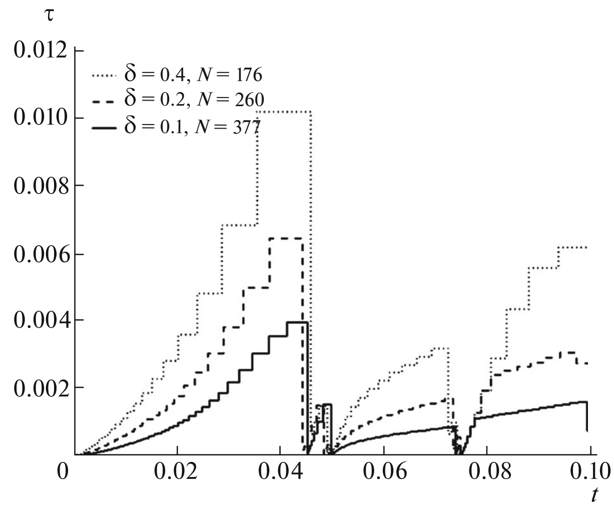

Fig. 7. Time steps in the three-level scheme used for prediction.

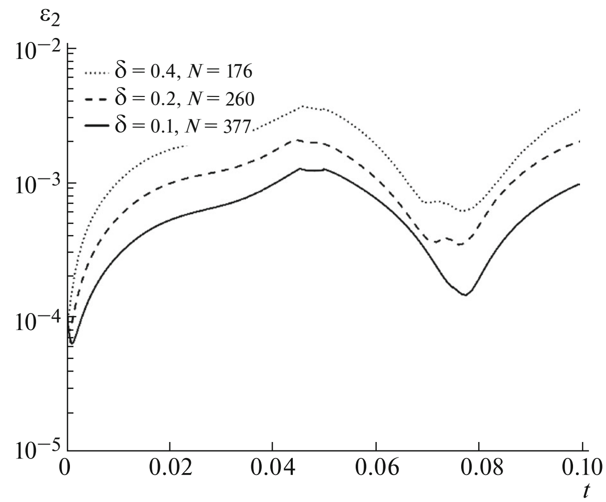

Fig. 8. Error in the three-level scheme used for prediction.

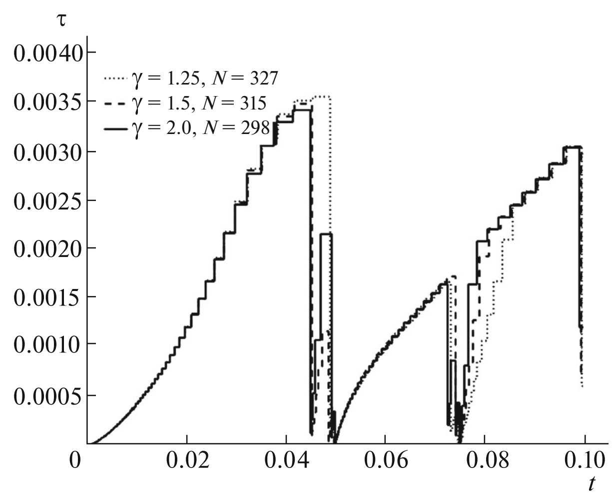

Fig. 9. Time steps for various γ.

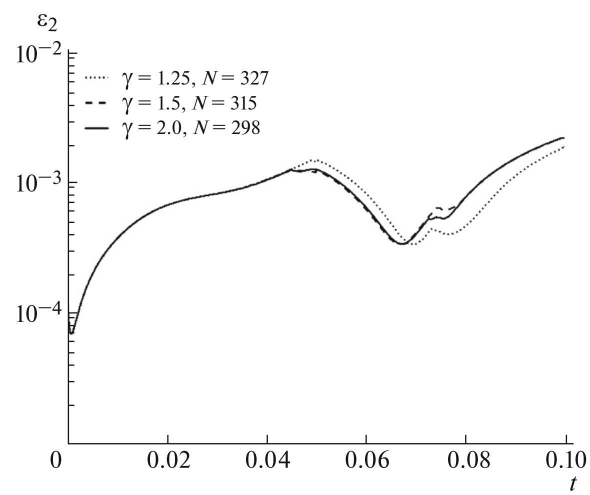

Fig. 10. Error for various γ.

As a test problem, we considered problem (4.1)–(4.3) with $T = 0.1$ and discontinuous functions $p(t)$ and $f(t)$:

$$p(t) = \begin{cases} \lambda t, & 0 < t \le 0.075, \\ 0, & 0.075 < t \le 0.1, \end{cases}$$

$$f(t) = \begin{cases} 0, & 0 < t \le 0.05, \\ \chi e^{-10(t-0.05)}, & 0.05 < t \le 0.1. \end{cases}$$

First, we consider the case where the initial condition (4.3) is specified as

$$u_0(x) = \sin^{\sigma}(\pi x), \quad 0 < x < 1.$$

For the basic version, we set

$$\lambda = 100, \quad \chi = 10, \quad \sigma = 0.5.$$

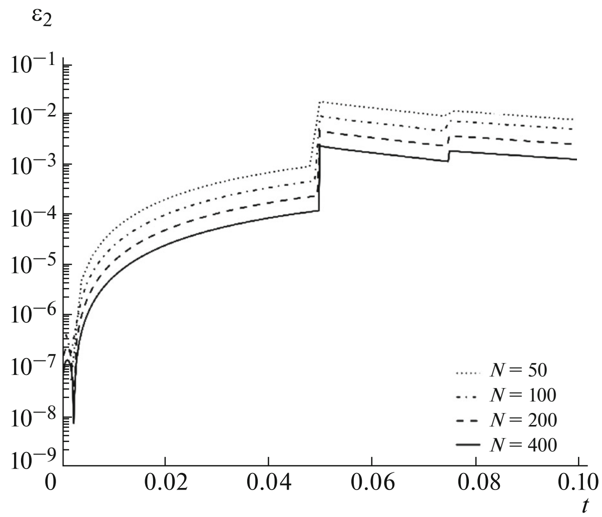

Fig. 11. Error on a uniform grid for $\sigma = 1$.

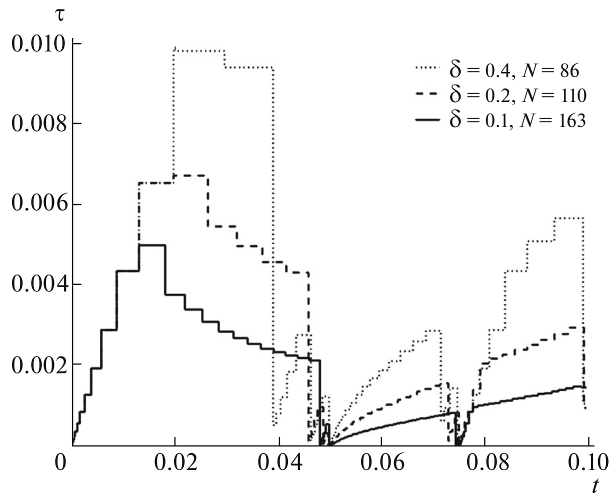

Fig. 12. Time steps for $\sigma = 1$.

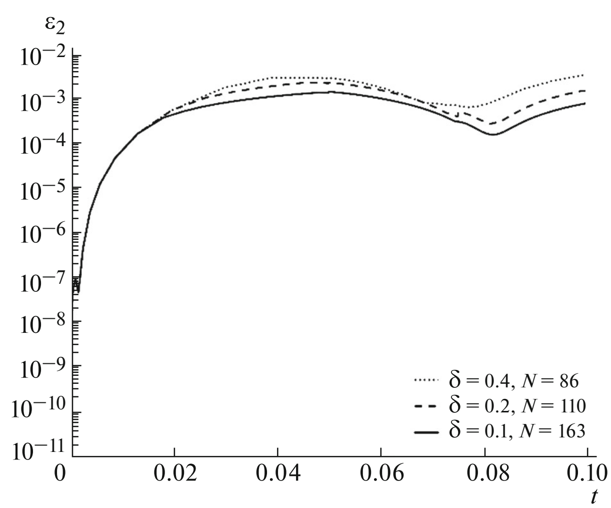

Fig. 13. Error for $\sigma = 1$.

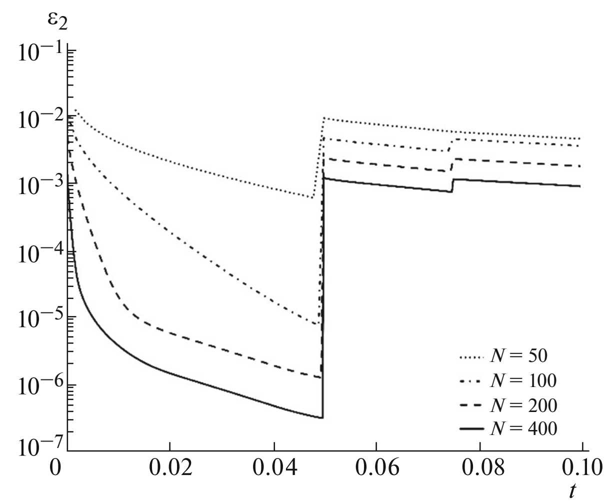

Fig. 14. Error on a uniform grid for the Crank–Nicolson scheme.

The problem was solved on a grid with $M = 100$. The computations were performed with a sufficiently small initial time step: $\tau_1 = \tau_0 = 1 \times 10^{-6}$. Since time approximation issues were addressed in this work, the spatial grid remained unchanged.

The accuracy of the approximate solution was estimated using a reference solution, namely, the numerical solution obtained on a fairly fine time grid (with $\tau = 1 \times 10^{-7}$). More specifically, the error was estimated in the $L_2(\omega)$ norm ($\varepsilon_2 = \|\cdot\|$) or in the $L_\infty(\omega)$ norm ($\varepsilon_\infty = \|\cdot\|_\infty$), where

$$\|u\|_\infty = \max_{x \in \omega} |u(x)|.$$

First, we discuss the errors of the approximate solutions obtained on uniform time grids. Figures 1 and 2 present the errors in the $L_2(\omega)$ and $L_\infty(\omega)$ norms, respectively. The plots show a high error at the beginning of the numerical process and its increase at $t = 0.05$ (discontinuity in $f(t)$) and at $t = 0.075$ (discontinuity in $p(t)$). A successful strategy for time step selection must capture these features: computa-

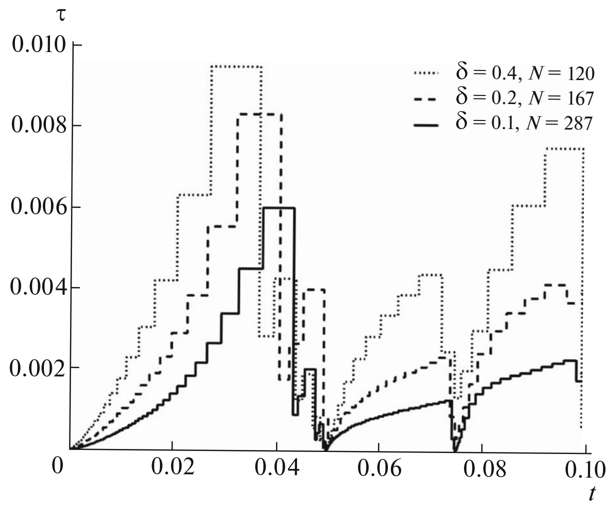

Fig. 15. Time steps in the Crank–Nicolson scheme.

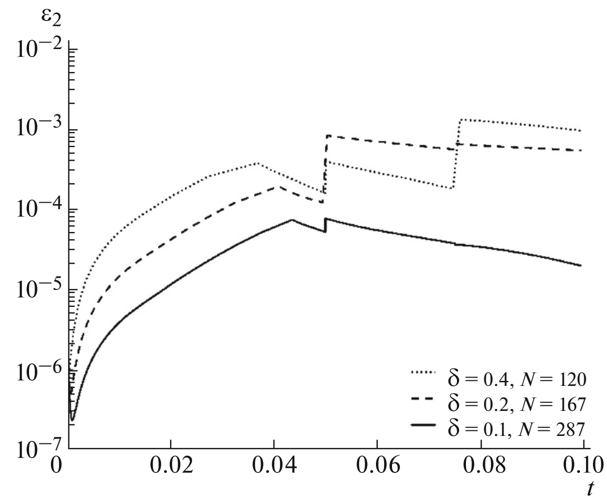

Fig. 16. Error for the Crank–Nicolson scheme.

tions have to be performed with a smaller time step in a right neighborhood of $t = 0$, $t = 0.05$, and $t = 0.075$.

The truncation error was determined using $T = 0.1$, and the approximate solution was found on a unit interval in x with a solution amplitude of order 1. Figure 3 shows the time steps determined according to (2.5) and (2.6) with the $L_2(\omega)$ norm used for estimating the truncation error. The parameter of time step increase was specified as $\gamma = 1.5$. The error obtained for various truncation errors is presented in Fig. 4. The computation starts with a small step, which is gradually increased, but then is reduced substantially near $t = 0.05$. A similar reduction in the time step is also observed near $t = 0.075$. The accuracy of the approximate solution increases considerably at short times. In fact, there is no loss of accuracy near the discontinuities in the right-hand side and the coefficient of the equation.

Similar results were obtained in the case of the $L_\infty(\omega)$ norm used in the truncation error estimation. Comparing Fig. 5 with Fig. 3 and Fig. 6 with Fig. 4, we see that the initial (minimum) step has to be reduced to improve the accuracy of the approximate solution for small t. Once again, the time step is changed significantly at $t = 0.05$ and $t = 0.075$, which correspond to discontinuities in the right-hand side and the coefficient of the equation. Thus, the time step selection algorithm performs well in the case of various norms used for truncation error estimation.

The prognostic solution is found using explicit scheme (2.3), which has the same (first) order of accuracy as implicit scheme (1.4). More accurate difference schemes might be used to find a prognostic solution. As an example, Figs. 7 and 8 presents the numerical results produced by the three-level explicit scheme (3.3). A comparison to the data obtained with explicit scheme (2.3) (see Figs. 3, 4) shows that the basic tendencies of time step selection and the accuracy achieved remain the same.

The basic parameters of the algorithm include γ, which is related to the choice of a prognostic time step. The results in Figs. 9 and 10 show that the influence of γ is insignificant.

Special attention was given to the influence exerted by the initial conditions, namely, by the parameter σ. A typical situation involves a boundary layer, which requires using a fine step at small times. For $\sigma = 1$, a better situation with the error is observed for small t (see Fig. 11). The nonuniform grid and the error in the approximate solution are presented in Figs. 12 and 13, respectively. In this case, the error is initially small, which is well reflected by the time step selection algorithm. The effect of the other parameters of the problem (λ and χ) is not very large.

Consider some numerical results produced by the second-order scheme (3.1) as applied to the model parabolic problem (4.1)–(4.3). Figure 14 shows the error of the approximate solution obtained on a uniform time grid. The time step selection algorithm (2.6), (3.5) is based on the three-level scheme (3.3). The resulting time step is shown in Fig. 15. The error of the approximate solution obtained on a nonuniform grid is illustrated in Fig. 16. A comparison of Figs. 15 and 14 shows that a far more accurate solution is obtained on sufficiently fine nonuniform time grids.

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