The two-level finite difference schemes for the heat equation with nonlocal initial condition

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Abstract

In this paper, the two-level finite difference schemes for the one-dimensional heat equation with a nonlocal initial condition are analyzed. As the main result, we obtain conditions for the numerical stability of the schemes. In addition, we revise the stability conditions obtained in [21] for the Crank–Nicolson scheme. We present several numerical examples that confirm the theoretical results within linear, as well as nonlinear problems. In some particular cases, it is shown that for small regions of the time step size values, the explicit FTCS scheme is stable while certain implicit methods, such as Crank–Nicolson scheme, are not.

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1. Introduction

Mathematical models arising in various fields of science and engineering very often are expressed in terms of partial differential equations (PDEs) with nonlocal initial or boundary conditions. For example, we can mention models arising in thermoelasticity [1], thermodynamics [2], geology [3], hydrodynamics [4], biological fluid dynamics [5] or plasma physics [6]. The present paper is focused on differential problems with *nonlocal initial conditions*. Such problems generalize the classical or time-periodic problems and can be seen as the control problems with initial conditions.

Nonclassical problems with nonlocal initial conditions are important because of their practical applications in modeling and investigation of sewage caused pollution processes in rivers and seas. Such problems are also used when investigating radionuclides propagation in Stokes fluid, diffusion and flow in porous media [7–9]. Nonlocal initial conditions also arise in mathematical models applied in meteorology since the use of time-averaged data instead of the initial data only leads to more reliable long-term weather forecasts [10].

In this paper, as a model problem we consider the one-dimensional parabolic (heat) equation

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = f(x,t), \quad (x,t) \in \Omega \times (0,T), \tag{1}$$

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subject to homogeneous boundary condition

$$u(x,t) = 0, \quad (x,t) \in \partial\Omega \times (0,T), \tag{2}$$

and nonlocal discrete–integral initial condition

$$u(x,0) = \sum_{j=1}^{m} \alpha_j u(x,T_j) + \int_0^T \upsilon(\tau) u(x,\tau)\mathrm{d}\tau + \varphi(x), \quad x \in \Omega. \tag{3}$$

Here $\Omega = (0,L)$ is a spatial interval, $\alpha_j \neq 0$, $0 < T_j \leq T$ $(1 \leq j \leq m)$, $\upsilon \in L^1(0,T)$.

Nonlocal in time problems for parabolic equations were considered in [11] and, later, in [7–9, 12–14] (see also references therein). The solvability of various differential problems with nonlocal initial conditions systematically has been studied in papers [15–18].

The existence and uniqueness results related to the problem (1)–(3) are given in paper [17]. If $\varphi \in L^2(\Omega)$, $f \in L^2([0,T]; H^{-1}(\Omega))$ and

$$1 - \sum_{j=1}^{m} \frac{\alpha_j + |\alpha_j|}{2} \geq \int_0^T |\upsilon(\tau)|\mathrm{d}\tau,$$

then the problem (1)–(3) has a unique solution $u \in C^0([0,T]; L^2(\Omega)) \cap L^2([0,T]; H_0^1(\Omega))$.

In recent decades, numerical methods for the solution of PDEs with nonlocal boundary conditions are developed and investigated very actively. However, only a few studies are related to the numerical solution of PDEs with nonlocal initial conditions. For example, the error estimates for the semidiscrete finite element approximation of the solution to linear parabolic equation have been obtained in paper [19]. Iterative finite element approximations of the solutions to parabolic equations with certain nonlocal initial conditions have been studied in [20]. For the numerical solution of nonlinear parabolic problems with a nonlocal initial condition, iterative finite difference schemes have been proposed and analyzed in [21, 22]. In papers [23, 24], the finite difference schemes for the one-dimensional parabolic (heat) equation with nonlocal discrete initial conditions were examined. For the solution of this problem, a polynomial-based collocation technique has been suggested in paper [25].

For the numerical solution of nonlinear parabolic problems with a nonlocal initial condition, and iterative finite difference scheme has been investigated in papers [21, 22]. In [21], the stability and convergence of several finite difference schemes have been studied.

In this paper, we extend the results presented in paper [21] to a more general class of methods, including numerical schemes which were applied previously without studying their stability properties. Additionally, we revise Theorem 3.2 proved in the paper [21] by adding a new constraint for the time step size. The revised analysis leads to the stability conditions which were not considered in [21, 23]. The numerical results presented in this paper show that conditions provided in [21, 23] cannot guarantee the stability of the corresponding numerical schemes. Also, we demonstrate that in some particular cases the forward-time central-space (FTCS) explicit numerical scheme is stable, while some implicit methods (such as Crank–Nicolson scheme) are not. From the point of view of the classical theory of finite difference schemes, this is a quite surprising result. The examined methods can be naturally extended for nonlinear problems. For illustration, we present the results of a numerical experiment with a nonlinear problem.

The paper is organized as follows. The two-level finite difference schemes for the solution of the considered nonclassical problem are presented in Section 2. In Section 3, we analyze these schemes by studying their stability and accuracy properties. To verify the theoretical results and demonstrate the efficiency of the methods, several numerical experiments have been conducted. The results of these experiments are presented in Section 4. Finally, some remarks in Section 5 conclude the paper.

2. Two-level finite difference schemes

For the numerical solution of the considered problem (1)–(2) we apply the finite difference technique [26–29]. We construct a family of finite difference schemes depending on several parameters.

The problem domain $\Omega \times [0, T]$ is discretized by the uniformly distributed grid points (x_i, t_n), where

$$
\begin{aligned}
&x_i = ih, \quad i = 0, 1, \ldots, N, \quad Nh = L,\\
&t_n = n\tau, \quad n = 0, 1, \ldots, M, \quad M\tau = T,
\end{aligned}
$$

where h and τ are space and time step sizes. We assume that $\{T_1, T_2, \ldots, T_m\} \subset \{t_0, t_1, \ldots, t_M\}$ and $T_j = t_{n_j}$ for some $n_j \in \{0, 1, \ldots, M\}$.

The one-dimensional parabolic equation (1) is approximated by the following finite difference equations:

$$
\begin{aligned}
\frac{u_i^{n+1} - u_i^n}{\tau} = \sigma \frac{u_{i-1}^{n+1} - 2u_i^{n+1} + u_{i+1}^{n+1}}{h^2} + (1 - \sigma)\frac{u_{i-1}^n - 2u_i^n + u_{i+1}^n}{h^2}\\
+ c_{00} f_{i-1}^{n+1} + c_{01} f_i^{n+1} + c_{00} f_{i+1}^{n+1} + c_{10} f_{i-1}^n + c_{11} f_i^n + c_{10} f_{i+1}^n,
\end{aligned} \tag{4}
$$

where σ is the weight of the scheme ($0 \le \sigma \le 1$), and c_{00}, c_{01}, c_{10}, c_{11} are coefficients to be determined later (see Section 3.2). Depending on the values of σ, we distinguish several special cases:

- $\sigma = 1$: the backward-time central-space (BTCS) scheme;
- $\sigma = 1/2$: the Crank–Nicolson scheme;
- $\sigma = 0$: the forward-time central-space (FTCS) scheme;
- $\sigma = 1/2 - 1/(12s)$, $s = \tau/h^2$: the Crandall's scheme.

The BTCS and Crank–Nicolson schemes are implicit, while the FTCS scheme is explicit. If $s = 1/6$, the Crandall's scheme also becomes explicit (otherwise, it is implicit).

From the homogeneous boundary condition (2) we have

$$
u_0^n = 0, \quad u_N^n = 0, \quad n = 0, 1, \ldots, M. \tag{5}
$$

The finite difference schemes are applied iteratively as it is explained in Section 3.3. For the initialization of the iterative procedure, we need initial guess of the initial values u_i^0. In each iteration, these values are updated using a discretized version of nonlocal initial condition (3) (see Section 3.3).

3. Analysis of the schemes

In this section, we analyze the stability of the finite difference schemes constructed in Section 2. We also obtain conditions ensuring the second or fourth order accuracy. Finally, we present an iterative procedure for the solution of the finite difference schemes.

3.1. Stability

We prove the stability of the considered numerical schemes by generalizing the idea used in [21, Theorem 3.1]. We will need an assumption similar to (H2) in [21]. Let us assume that

$$
\sum_{n=1}^{M} |\widetilde{\alpha}_n| \exp\{-t_n \lambda_{\min}\} = \varrho < 1. \tag{H}
$$

We define the $(N-1)\times(N-1)$ matrix

$$\mathbf{\Lambda} = h^{-2}\begin{pmatrix} 2 & -1 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 2 & \ddots & 0 & 0 & 0 \\ \cdots & \cdots & \ddots & \ddots & \ddots & \cdots & \cdots \\ 0 & 0 & 0 & \ddots & 2 & -1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 2 & -1 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 2 \end{pmatrix}$$

and rewrite the finite difference equations (4) in the following form:

$$(\mathbf{I} + \sigma\tau\mathbf{\Lambda})U^{n+1} = (\mathbf{I} - (1-\sigma)\tau\mathbf{\Lambda})U^n + \tau F^{n+1}, \tag{6}$$

where $\mathbf{I}$ is the identity matrix of order $N-1$, $U = (u_1, u_2, \ldots, u_{N-1})^T$ is unknown vector, and F^{n+1} is given $(N-1)$-dimensional vector. From (6) it follows that

$$U^{n+1} = \mathbf{S}U^n + \overline{F}^{n+1},$$

where

$$\mathbf{S} = (\mathbf{I} + \sigma\tau\mathbf{\Lambda})^{-1}(\mathbf{I} - (1-\sigma)\tau\mathbf{\Lambda}), \quad \overline{F}^{n+1} = \tau(\mathbf{I} + \sigma\tau\mathbf{\Lambda})^{-1}F^{n+1}.$$

Thus, we obtain that

$$U^n = \mathbf{S}^n U^0 + \sum_{m=0}^{n} \mathbf{S}^{n-m}\overline{F}^m.$$

It is well-known that the eigenvalues of the matrix $\mathbf{\Lambda}$ are real, positive and algebraically simple numbers [30]:

$$\lambda_i(\mathbf{\Lambda}) = \frac{4}{h^2}\sin^2\Big(\frac{i\pi h}{2}\Big), \quad i = 1, 2, \ldots, N-1.$$

Therefore,

$$\lambda_{\min} := \min_{i=1,2,\ldots,N-1} \lambda_i(\mathbf{\Lambda}) = \lambda_1(\mathbf{\Lambda}) = \pi^2 - \varepsilon_{1,h},$$

and

$$\lambda_{\max} := \max_{i=1,2,\ldots,N-1} \lambda_i(\mathbf{\Lambda}) = \lambda_{N-1}(\mathbf{\Lambda}) = 4(N-1)^2 - \varepsilon_{2,h},$$

where $\varepsilon_{1,h}$ and $\varepsilon_{2,h}$ are positive constants ($\varepsilon_{1,h}, \varepsilon_{2,h} \to 0$, when $h \to 0$).

The eigenvalues of the matrix $\mathbf{S}$ can be expressed as

$$\lambda_i(\mathbf{S}) = \frac{1 - (1-\sigma)\tau\lambda_i(\mathbf{\Lambda})}{1 + \sigma\tau\lambda_i(\mathbf{\Lambda})}, \quad i = 1, 2, \ldots, N-1,$$

Then

$$\|\mathbf{S}\| = \|(\mathbf{I} + \sigma\tau\mathbf{\Lambda})^{-1}(\mathbf{I} - (1-\sigma)\tau\mathbf{\Lambda})\| \leq \max_{i=1,2,\ldots,N-1} \left| \frac{1-(1-\sigma)\tau\lambda_i(\mathbf{\Lambda})}{1+\sigma\tau\lambda_i(\mathbf{\Lambda})} \right| = \rho(\mathbf{S}),$$

and the inequality $\|\mathbf{S}\| < 1$ is ensured, if

$$\sigma > \frac{1}{2} - \frac{1}{\tau\rho(\mathbf{\Lambda})},$$

where $\rho(\mathbf{\Lambda})$ is the spectral radius of the matrix $\mathbf{\Lambda}$:

$$\rho(\mathbf{\Lambda}) = \frac{4}{h^2}\cos^2\Big(\frac{\pi h}{2}\Big).$$

The inequality $\|\mathbf{S}\| < 1$ is enough to guarantee the stability of the finite difference scheme for the problem with a classical initial condition. However, in the case of nonlocal initial condition, this is not always the case.

In paper [21], the spectral radius of the matrix $\mathbf{S}$ is defined as

$$\rho(\mathbf{S}) = \frac{1-(1-\sigma)\tau\lambda_{\min}}{1+\sigma\tau\lambda_{\min}}, \tag{7}$$

i.e., the absolute value $|\cdot|$ is not used in the definition of $\rho(\mathbf{S})$. Under this assumption, the unconditional stability of the Crank–Nicolson scheme is proved (see [21, Theorem 3.2]). However, as we will theoretically prove and demonstrate in numerical examples, the Crank–Nicolson scheme for the problem with the nonlocal initial condition is not unconditionally stable.

Let us study the stability under the assumption that (7) holds true. Below we demonstrate in which cases (7) is not correct and formulate additional conditions that are required for the stability and, consequently, convergence.

If the spectral radius of the matrix $\mathbf{S}$ is defined by (7), we obtain that

$$\|U^n\| \leq \Big(\frac{1-(1-\sigma)\tau\lambda_{\min}}{1+\sigma\tau\lambda_{\min}}\Big)^n \|U^0\| + \sum_{m=0}^{n} \Big(\frac{1-(1-\sigma)\tau\lambda_{\min}}{1+\sigma\tau\lambda_{\min}}\Big)^{n-m} \|\overline{F}^m\|.$$

The elementary inequality

$$\frac{1}{1+v} < \exp\Big\{-\frac{v}{1+v}\Big\}, \quad v > 0,$$

can be applied here. Hence, if we assume that v is such that

$$\frac{1}{1+v} = \frac{1-(1-\sigma)\tau\lambda_{\min}}{1+\sigma\tau\lambda_{\min}},$$

i.e. $v = \tau\lambda_{\min}/(1-(1-\sigma)\tau\lambda_{\min})$ and $\tau\lambda_{\min}/(1-(1-\sigma)\tau\lambda_{\min}) > 0$, then

$$\sigma > 1 - \frac{1}{\tau\lambda_{\min}}.$$

We can easily check that

$$\Big(\frac{1-(1-\sigma)\tau\lambda_{\min}}{1+\sigma\tau\lambda_{\min}}\Big)^n < \Big(\exp\Big\{-\frac{\tau\lambda_{\min}}{1+\sigma\tau\lambda_{\min}}\Big\}\Big)^n = \exp\Big\{-\frac{t_n\lambda_{\min}}{1+\sigma\tau\lambda_{\min}}\Big\}.$$

Actually, since

$$-\frac{t_n\lambda_{\min}}{1+\sigma\tau\lambda_{\min}} = -t_n\lambda_{\min}(1-\sigma\tau\lambda_{\min}+\cdots) \le -t_n\lambda_{\min} + T\sigma\tau\lambda_{\min}^2,$$

for small τ, we obtain that

$$\Big(\frac{1-(1-\sigma)\tau\lambda_{\min}}{1+\sigma\tau\lambda_{\min}}\Big)^n < \exp\{-t_n\lambda_{\min}\}\exp\{T\sigma\tau\lambda_{\min}^2\}.$$

By using the expression above and the initial condition (12) it is easy to verify that

$$\begin{aligned}\|U^0\| &\le \sum_{n=1}^{M}(|\widetilde{\alpha}_n|\cdot\|U^n\|) + \|\Phi\| \\ &\le \sum_{n=1}^{M}|\widetilde{\alpha}_n|\exp\{-t_n\lambda_{\min}\}\exp\{T\sigma\tau\lambda_{\min}^2\}\|U^0\| + \sum_{m=0}^{n}\|\overline{F}^m\| + \|\Phi\|,\end{aligned}$$

where $\Phi = (\varphi(x_1),\ldots,\varphi(x_{N-1}))^T$. Assuming (H), there exists $\tau_0 = -\log\varrho/(T\sigma\lambda_{\min}^2) > 0$ such that

$$\|U^0\| \le C\Big[\sum_{m=0}^{n}\|\overline{F}^m\| + \|\Phi\|\Big]$$

for all $0 < \tau \le \tau_0$.

Finally, let us check when

$$\rho(\mathbf{S}) = \frac{1-(1-\sigma)\tau\lambda_{\min}}{1+\sigma\tau\lambda_{\min}}.$$

It is clear that the function

$$\overline{f}(\tau\lambda) := \frac{1-(1-\sigma)\tau\lambda}{1+\sigma\tau\lambda}$$

decreases when $\tau\lambda$ increases since its derivative with respect to $\tau\lambda$ is

$$-\frac{1}{(1+\tau\lambda\sigma)^2} < 0,$$

and $\overline{f}(\tau\lambda) \to 1$ when $\tau\lambda \to 0$. Hence, if $0 \le \sigma \le 1$, then

$$\frac{1-(1-\sigma)\tau\lambda_{\min}}{1+\sigma\tau\lambda_{\min}}$$

is positive whenever $\tau < 1/\lambda_{\min}$, and

$$\max_{i=1,2,\ldots,N-1}\Big|\frac{1-(1-\sigma)\tau\lambda_i(\mathbf{\Lambda})}{1+\sigma\tau\lambda_i(\mathbf{\Lambda})}\Big| = \max\Big(\frac{1-(1-\sigma)\tau\lambda_{\min}}{1+\sigma\tau\lambda_{\min}}, -\frac{1-(1-\sigma)\tau\lambda_{\max}}{1+\sigma\tau\lambda_{\max}}\Big).$$

It is also clear that

$$-\frac{1-(1-\sigma)\tau\lambda_{\max}}{1+\sigma\tau\lambda_{\max}} \le \frac{1-(1-\sigma)\tau\lambda_{\min}}{1+\sigma\tau\lambda_{\min}}, \tag{8}$$

if

$$0 < \tau \le \tau_0^* = \frac{\gamma(1-2\sigma) - \sqrt{\gamma^2(1-2\sigma)^2 - 16\lambda_{\min}\lambda_{\max}\sigma(\sigma-1)}}{4\lambda_{\min}\lambda_{\max}\sigma(\sigma-1)},$$

where $\gamma = \lambda_{\min} + \lambda_{\max}$. Additionally, the left-hand side of inequality (8) decreases when σ increases, while the right-hand side increases when σ increases. Hence, if $0 \le \sigma \le 1$, the most restrictive case (for the inequality (8)), as it is expected, is $\sigma = 0$ and it holds whenever $\tau \le 2/\gamma$.

Under the assumption (H), we prove the following theorem:

Theorem 1. *If $0 < \sigma \le 1$, then there exists a constant $C > 0$ independent on τ and h such that*

$$\max_{0\le n\le M} \|U^n\| \le C\Big(\sum_{m=0}^{n} \|\overline{F}^m\| + \|\Phi\|\Big) \tag{9}$$

for all $0 < \tau \le \tau_0 = \min\left(-\log\varrho/(T\sigma\lambda_{\min}^2), \tau_0^*\right)$.

Consequently, we obtain corollaries for the various finite difference schemes described in Section 2.

Corollary 2. *If $\sigma = 1$ (BTCS scheme), then there exists constant $C > 0$ independent on τ and h such that the estimate (9) is valid for all $0 < \tau \le \tau_0 = -\log\varrho/(T\lambda_{\min}^2)$.*

This result is similar to the one obtained in [21], but in this case (when $\sigma = 1$), (8) holds for any value of τ.

Corollary 3. *If $\sigma = 1/2$ (Crank–Nicolson scheme), then there exists constant $C > 0$ independent on τ and h such that the estimate (9) is valid for all $0 < \tau \le \tau_0 = 2\min\left(-\log\varrho/(T\lambda_{\min}^2), 1/\sqrt{\lambda_{\min}\lambda_{\max}}\right)$.*

The stability condition the Crank–Nicolson scheme is different from the one obtained in [21]. Moreover, in the paper [23] it is stated that the Crank–Nicolson scheme for the heat equation with the nonlocal initial condition is unconditionally stable in the sense of von Neumann. In fact, the nonlocal initial condition affects the stability of the Crank–Nicolson scheme.

Corollary 4. *If $\sigma = 1/2 - 1/(12s)$, $s = \tau/h^2$ (Crandall's scheme), then there exists constant $C > 0$ independent on τ and h such that the estimate (9) is valid for all $0 < \tau \le \tau_0 = \min\left(-\log\varrho/(T\sigma\lambda_{\min}^2), \widehat{\tau}_0\right)$, where*

$$\widehat{\tau}_0 = \frac{6s\Big(\lambda_{\min} + \lambda_{\max} - \sqrt{(\lambda_{\min}-\lambda_{\max})^2 + 144\lambda_{\min}\lambda_{\max}s^2}\Big)}{\lambda_{\min}\lambda_{\max}(1-36s^2)}. \tag{10}$$

Remark 5. In Corollary 4, $\widehat{\tau}_0$ is given as a function depending on $s = \tau/h^2$. Given T and h (and, therefore, $\lambda_{\min}$ and $\lambda_{\max}$), it is possible to obtain the bound $\widehat{\tau}_0$ by substituting s with $\widehat{\tau}_0/h^2$ in (10) and solving a nonlinear equation.

Corollary 6. *If $\sigma = 0$ (FTCS scheme), then there exists $C > 0$ independent on τ and h such that the estimate (9) is valid for all $0 < \tau \le \tau_0 = 2/(\lambda_{\min} + \lambda_{\max})$.*

Corollary 7. *There exists $C > 0$ independent on τ and h such that the estimate (9) is valid for all $0 < \tau \le \tau_0 = -\log\varrho/(T\sigma\lambda_{\min}^2)$, whenever*

$$\sigma > \frac{\lambda_{\min}\lambda_{\max}\tau_0 - \gamma - \sqrt{(\lambda_{\min}-\lambda_{\max})^2 + (\lambda_{\min}\lambda_{\max}\tau_0)^2}}{2\gamma\tau_0}.$$

Remark 8. Similarly as in Corollary 4, τ_0 is given as a function depending on σ, where σ satisfies condition depending on τ_0. Given ϱ, T and h (and, therefore, $\lambda_{\min}$, $\lambda_{\max}$ and γ), one can obtain the bound for τ_0, by substituting σ with the expression depending on τ_0 and solving a nonlinear equation.

3.2. Accuracy

By using Taylor series in (4), taking $\tau = sh^2$ (for a fixed value of s) and

$$u_t - u_{xx} - f \equiv 0,$$

(i.e. it is also necessary to consider that $u_{tt} - u_{txx} - f_t = 0$, $u_{tx} - u_{xxx} - f_x = 0, \ldots$), we obtain the local truncation error of the finite difference equations:

$$\begin{aligned}
&-(2c_{00} + c_{01} + 2c_{10} + c_{11} - 1)f \\
&+(1/12)\left(-6(2c_{00} + 2c_{10} - s + 2s\sigma)f_{xx} + (-1 + 6s - 12s\sigma)u_{xxxx} - 6(-1 + 4c_{00} + 2c_{01})sf_t\right)h^2 + O(h^4).
\end{aligned}$$

In order to achieve the second order accuracy, it is necessary that coefficients $c_{00}, c_{01}, c_{10}, c_{11}$ would satisfy condition

$$2c_{00} + c_{01} + 2c_{10} + c_{11} - 1 = 0. \tag{11}$$

Additionally, if we aim to achieve the fourth order accuracy, it is necessary to add three more conditions:

$$\begin{aligned}
&2c_{00} + 2c_{10} - s + 2s\sigma = 0, \\
&1 - 6s + 12s\sigma = 0, \\
&(-1 + 4c_{00} + 2c_{01})s = 0.
\end{aligned}$$

Explicit schemes for the solution of linear problems are obtained with $\sigma = 0$. In the case of nonlinear problems, we need $c_{00} = 0$ and $c_{01} = 0$ (otherwise, one needs to solve a nonlinear system in each iteration). Obviously, from (4) it is not possible to obtain an explicit fourth order scheme for nonlinear problems, but the second order accuracy is possible.

In a similar way, the fourth order finite difference schemes have been derived and applied to solve PDEs with nonlocal boundary conditions [31–33].

Remark 9. Above we imposed $\tau = sh^2$ for a fixed s to the finite difference equations given in (4) (many of the methods used in Section 4 require this condition in order to obtain an optimal convergence). When (11) is also satisfied, this is enough to obtain the second order accuracy. However, the convergence of the methods proposed below can be very different: while the truncation error of BTCS and FTC schemes is $O(\tau + h^2)$, for Crank–Nicolson scheme it is $O(\tau^2 + h^2)$. Hence, this method is often applied with $\tau = sh$.

3.3. Implementation of the iterative solution procedure

The numerical schemes are applied iteratively. First of all, we discretize the nonlocal initial condition (3) in the following way:

$$(u_i^0)^{(l+1)} = \sum_{j=1}^{m} \alpha_j (u_i^{n_j})^{(l)} + \tau \sum_{n=0}^{M} w_n v(t_n)(u_i^n)^{(l)} + \varphi(x_i), \quad i = 1, 2, \ldots, N-1,$$

i.e.

$$(u_i^0)^{(l+1)} = \sum_{n=0}^{M} \widetilde{\alpha}_n (u_i^n)^{(l)} + \varphi(x_i), \quad i = 1, 2, \ldots, N-1, \tag{12}$$

where

$$\widetilde{\alpha}_n = \begin{cases} \tau w_n \upsilon(t_n) + \alpha_n, & \text{if } t_n \in \{T_1, T_2, \dots, T_m\}, \\ \tau w_n \upsilon(t_n), & \text{otherwise}, \end{cases}$$

real positive numbers w_n are the coefficients of the numerical integration formula, and l is the iteration number. For example, in case of the second order composite formula (trapezoid rule) we have $w_0 = w_M = 1/2$, $w_1 = w_2 = \cdots = w_{M-1} = 1$, and for the fourth order composite formula $w_0 = w_M = 1/3$, $w_1 = w_3 = \ldots = w_{M-1} = 4/3$, $w_2 = w_4 = \ldots = w_{M-2} = 2/3$ (M is even). If the sixth order composite formula is applied, then $w_0 = w_M = 7\widetilde{w}$, $w_1 = w_3 = \ldots = w_{M-1} = 32\widetilde{w}$, $w_2 = w_6 = \ldots = w_{M-2} = 12\widetilde{w}$, $w_4 = w_8 = \ldots = w_{M-4} = 14\widetilde{w}$, where $\widetilde{w} = 2/45$ (M is a multiple of 4).

The iterative solution procedure is executed in the following way:

Step 1: The initial guess is set to be $(u_i^0)^{(0)} = 0$, $i = 0, 1, \dots, N$.

Step 2: The values $(u_i^n)^{(l)}$ are computed using numerical scheme (4) and (5) (l is the number of current iteration).

Step 3: If the termination criterion

$$\|(u_i^0)^{(l)} - (u_i^0)^{(l-1)}\| \leq \text{TOL}$$

is not satisfied (TOL is a prescribed tolerance; in our experiments, $\text{TOL} = 0.1h^p$, p is the order of the method), the next iteration (Step 2) is executed with initial values updated using discretized nonlocal initial condition.

The iterative procedure can be applied to solve not only nonlocal linear heat equation but a nonlinear one too. This is one important advantage of iterative finite difference methods (see [21]) with respect to, for example, spectral or pseudo-spectral methods [34]. However, in a nonlinear case also it would be necessary to study the stability of the scheme and the stability conditions can be different.

4. Numerical examples

To justify the theoretical results and investigate the efficiency of the considered numerical schemes, we have analyzed several test examples, including an illustrative example of a nonlinear problem. In this section, we present and discuss the results.

4.1. Technical details

In our experiments, we applied four numerical schemes with different integration rules:

Scheme 1: $\sigma = 1$, BTCS, $c_{01} = 1$, $c_{00} = c_{10} = c_{11} = 0$, trapezoid formula ($p = 2$);

Scheme 2: $\sigma = 1/2$, Crank–Nicolson, $c_{00} = c_{10} = 0$, $c_{01} = c_{11} = 1/2$, trapezoid formula ($p = 2$);

Scheme 3: $\sigma = 0$, $s = 1/6$, an explicit Crandall's method, $c_{00} = 1/12$, $c_{01} = 1/3$, $c_{10} = 0$, $c_{11} = 1/2$, Simpson's composite formula ($p = 4$);

Scheme 4: $\sigma = 0$, FTCS, $c_{00} = c_{01} = c_{10} = 0$, $c_{11} = 1$, trapezoid formula ($p = 2$).

Schemes 1 and 2 are implicit, while Schemes 3 and 4 are explicit.

The accuracy of the methods applied in the numerical examples was estimated by calculating absolute errors in the last iteration

$$E = |u(x_i, t_n) - u_i^n|$$

on certain points x_i and time moments t_n, or the maximum norm of the absolute error

$$E_\infty = \max_{\substack{0\le i\le N\\ 0\le n\le M}} |u(x_i,t_n) - u_i^n|.$$

All numerical examples are formulated on the unit spatial interval ($\Omega = (0,1)$, i.e. $L = 1$).

4.2. Test 1: Problem with nonlocal discrete initial condition

In the first example, we consider the problem with nonlocal discrete initial condition ($\upsilon(t) \equiv 0$) [23–25]. The functions $f(x,t)$ and $\varphi(x)$ are chosen so that the function

$$u(x,t) = \sin(\pi x)\exp(-t)$$

is the exact solution of the problem, i.e.

$$f(x,t) = (\pi^2 - 1)\sin(\pi x)\exp(-t),$$
$$\varphi(x) = -\sin(\pi x)\sum_{j=1}^{m}\alpha_j \exp(-T_j).$$

We set $m = 2$ and $T_1 = 0.5$, $T_2 = T = 1$, $\alpha_1 = -\alpha_2 = 1$.

Numerical results are reported in Table 1. Schemes 1 and 2 demonstrate the accuracy of the second order, while the accuracy of the Scheme 3 is of the order four.

4.3. Test 2: Problem with nonlocal discrete–integral initial condition

The second test example involves an integral term in the nonlocal initial condition ($\upsilon(t) \equiv 1$). We choose $T = 1$, $m = 4$ and $\alpha_j = -1$, $T_j = j/m$ for $1 \le j \le m$. If

$$f(x,t) = \frac{4\pi}{1+t}(4\pi x^2\sin(2\pi x^2) - \cos(2\pi x^2)) - \frac{\sin(2\pi x^2)}{(1+t)^2},$$
$$\varphi(x) = \sin(2\pi x^2)\Big(1 - \sum_{j=1}^{m}\frac{\alpha_j}{1+T_j} - \log(1+T)\Big),$$

then the exact solution of the problem is

$$u(x,t) = \frac{\sin(2\pi x^2)}{1+t}.$$

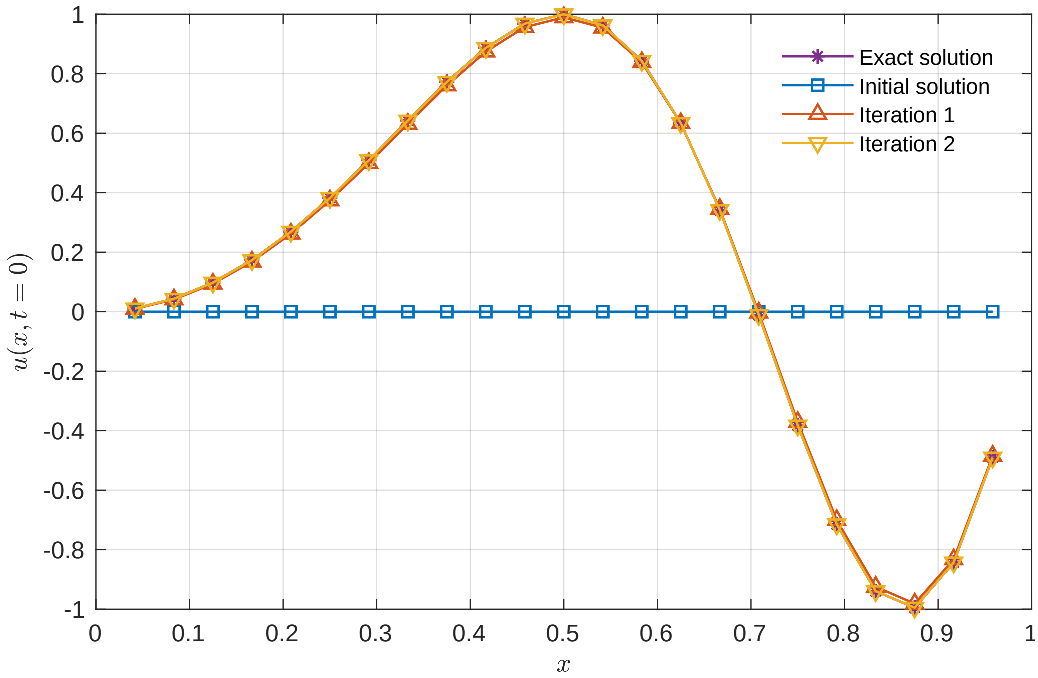
The results are reported in Fig. 1 and Table 2. In Fig. 1 we present the numerical approximation of initial values $u(x,0)$ obtained in first two iterations of Scheme 3. The orders of accuracy for Schemes 1–3 are presented in Table 2 and they are the same as in the previous example. However, the iterative procedure requires more iterations in order to achieve the prescribed accuracy.

Table 1
Absolute errors ($t = 1$, $x = 0.25, 0.5$ and 0.75), order of accuracy and the total number of iterations required to achieve the prescribed accuracy: Test 1, $\tau = sh^2$ ($s = 4$ for Schemes 1 and 2, $s = 1/6$ for Scheme 3)

	Errors			Order	Number of iterations
	$x = 0.25$	$x = 0.5$	$x = 0.75$		
Scheme 1					
$h = 1/20$	$7.43804 \cdot 10^{-4}$	$1.0519 \cdot 10^{-3}$	$7.43804 \cdot 10^{-4}$	–	3
$h = 1/40$	$1.85561 \cdot 10^{-4}$	$2.62423 \cdot 10^{-4}$	$1.85561 \cdot 10^{-4}$	~ 2.00303	3
$h = 1/80$	$4.63666 \cdot 10^{-5}$	$6.55723 \cdot 10^{-5}$	$4.63666 \cdot 10^{-5}$	~ 2.00188	4
$h = 1/160$	$1.15901 \cdot 10^{-6}$	$1.63909 \cdot 10^{-5}$	$1.15901 \cdot 10^{-6}$	~ 2.00132	4
$h = 1/320$	$2.89742 \cdot 10^{-6}$	$4.09758 \cdot 10^{-6}$	$2.89742 \cdot 10^{-6}$	~ 2.001	4
Scheme 2					
$h = 1/20$	$5.95736 \cdot 10^{-4}$	$8.42497 \cdot 10^{-4}$	$5.95735 \cdot 10^{-4}$	–	2
$h = 1/40$	$1.48814 \cdot 10^{-4}$	$2.10456 \cdot 10^{-4}$	$1.48814 \cdot 10^{-4}$	~ 2.00115	3
$h = 1/80$	$3.71968 \cdot 10^{-5}$	$5.26043 \cdot 10^{-5}$	$3.71968 \cdot 10^{-5}$	~ 2.00071	4
$h = 1/160$	$9.29874 \cdot 10^{-6}$	$1.31504 \cdot 10^{-5}$	$9.29874 \cdot 10^{-6}$	~ 2.0005	4
$h = 1/320$	$2.32464 \cdot 10^{-6}$	$3.28755 \cdot 10^{-6}$	$2.32464 \cdot 10^{-6}$	~ 2.00038	4
Scheme 3					
$h = 1/12$	$6.53692 \cdot 10^{-6}$	$9.24461 \cdot 10^{-6}$	$6.53692 \cdot 10^{-6}$	–	4
$h = 1/24$	$4.07833 \cdot 10^{-7}$	$5.76763 \cdot 10^{-7}$	$4.07833 \cdot 10^{-7}$	~ 4.00256	5
$h = 1/48$	$2.54782 \cdot 10^{-8}$	$3.60316 \cdot 10^{-8}$	$2.54782 \cdot 10^{-8}$	~ 4.0016	5
$h = 1/96$	$1.59233 \cdot 10^{-9}$	$2.25189 \cdot 10^{-9}$	$1.59233 \cdot 10^{-9}$	~ 4.00109	6
$h = 1/192$	$9.99528 \cdot 10^{-11}$	$1.41368 \cdot 10^{-10}$	$9.99524 \cdot 10^{-11}$	~ 3.99922	6

Table 2
Absolute errors ($t = 1$, $x = 0.25, 0.5$ and 0.75), order of accuracy and the total number of iterations required to achieve the prescribed accuracy: Test 2, $\tau = sh^2$ ($s = 4$ for Schemes 1 and 2, $s = 1/6$ for Scheme 3).

	Errors			Order	Number of iterations
	$x = 0.25$	$x = 0.5$	$x = 0.75$		
Scheme 1					
$h = 1/20$	$6.77636 \cdot 10^{-4}$	$5.75261 \cdot 10^{-3}$	$7.68408 \cdot 10^{-4}$	–	4
$h = 1/40$	$1.62955 \cdot 10^{-4}$	$1.41878 \cdot 10^{-3}$	$2.24531 \cdot 10^{-4}$	~ 2.01956	4
$h = 1/80$	$4.03533 \cdot 10^{-5}$	$3.5352 \cdot 10^{-4}$	$5.80869 \cdot 10^{-5}$	~ 2.01218	4
$h = 1/160$	$1.00645 \cdot 10^{-5}$	$8.83068 \cdot 10^{-5}$	$1.46428 \cdot 10^{-5}$	~ 2.00852	5
$h = 1/320$	$2.51464 \cdot 10^{-6}$	$2.20721 \cdot 10^{-5}$	$3.66824 \cdot 10^{-6}$	~ 2.00646	5
Scheme 2					
$h = 1/20$	$6.16576 \cdot 10^{-4}$	$5.66897 \cdot 10^{-3}$	$8.0206 \cdot 10^{-4}$	–	4
$h = 1/40$	$1.47886 \cdot 10^{-4}$	$1.39819 \cdot 10^{-3}$	$2.32869 \cdot 10^{-4}$	~ 2.01952	4
$h = 1/80$	$3.65987 \cdot 10^{-5}$	$3.48391 \cdot 10^{-4}$	$6.01665 \cdot 10^{-5}$	~ 2.01215	4
$h = 1/160$	$9.12664 \cdot 10^{-6}$	$8.70259 \cdot 10^{-5}$	$1.51623 \cdot 10^{-5}$	~ 2.0085	5
$h = 1/320$	$2.28022 \cdot 10^{-6}$	$2.1752 \cdot 10^{-5}$	$3.79811 \cdot 10^{-6}$	~ 2.00645	5
Scheme 3					
$h = 1/12$	$2.79303 \cdot 10^{-4}$	$8.23333 \cdot 10^{-4}$	$1.41436 \cdot 10^{-3}$	–	5
$h = 1/24$	$1.57131 \cdot 10^{-5}$	$4.82578 \cdot 10^{-5}$	$8.14607 \cdot 10^{-5}$	~ 4.09264	5
$h = 1/48$	$9.56521 \cdot 10^{-7}$	$2.96915 \cdot 10^{-6}$	$4.98878 \cdot 10^{-6}$	~ 4.05764	6
$h = 1/96$	$5.93899 \cdot 10^{-8}$	$1.8485 \cdot 10^{-7}$	$3.10219 \cdot 10^{-7}$	~ 4.0403	7
$h = 1/192$	$3.70605 \cdot 10^{-9}$	$1.15423 \cdot 10^{-8}$	$1.93642 \cdot 10^{-8}$	~ 4.03057	8



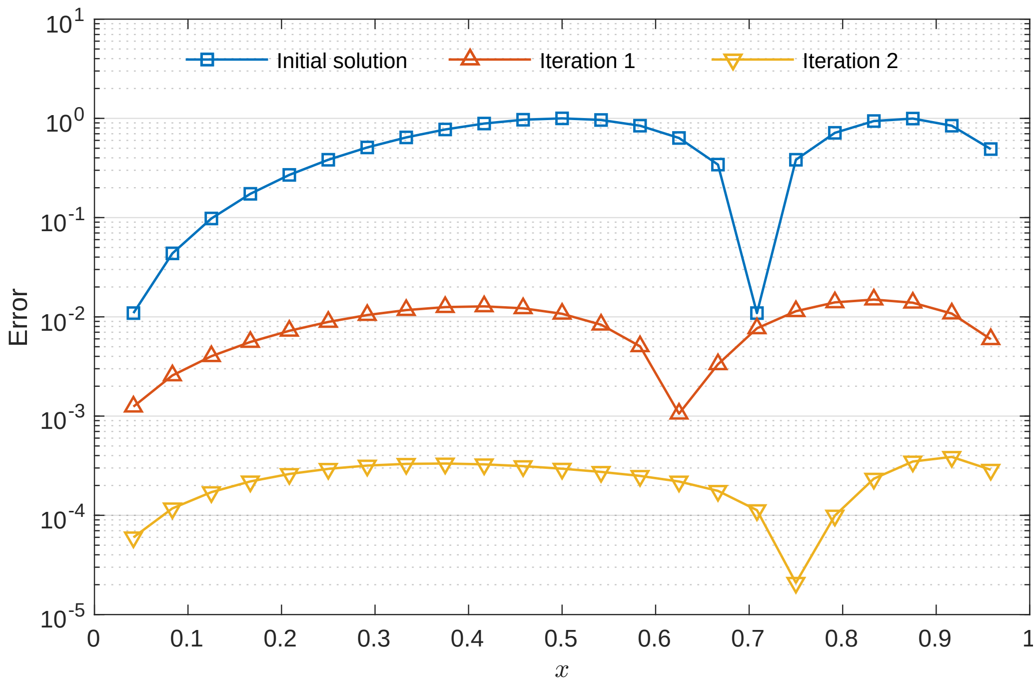


Fig. 1. Numerical approximation of the initial value $u(x, t = 0)$ at the initialization and after the first two iterations: Test 2, Scheme 3, $\tau = sh^2$, $s = 1/6$, $h = 1/24$; approximate values (top) and absolute errors (bottom).

Table 3
Maximum norms of the absolute error (E_∞): Test 3, Scheme 2, $h = 1/400$.

	Errors E_∞		
Iteration	$\tau = 1/200$	$\tau = 1/1000$	$\tau = 1/2000$
1	$9.996716 \cdot 10^{-1}$	$1.047698 \cdot 10^{0}$	$1.053871 \cdot 10^{0}$
2	$1.297642 \cdot 10^{-3}$	$1.351188 \cdot 10^{-3}$	$1.357894 \cdot 10^{-3}$
3	$5.946431 \cdot 10^{-4}$	$2.587616 \cdot 10^{-5}$	$2.608255 \cdot 10^{-5}$
4	$3.209209 \cdot 10^{-3}$	$2.404325 \cdot 10^{-5}$	$2.424209 \cdot 10^{-5}$
5	$1.909528 \cdot 10^{-2}$	$2.404579 \cdot 10^{-5}$	$2.424464 \cdot 10^{-5}$
6	$1.202271 \cdot 10^{-1}$	$2.404579 \cdot 10^{-5}$	$2.424464 \cdot 10^{-5}$
7	$7.857214 \cdot 10^{-1}$	$2.404579 \cdot 10^{-5}$	$2.424464 \cdot 10^{-5}$
8	$5.273521 \cdot 10^{0}$	$2.404579 \cdot 10^{-5}$	$2.424464 \cdot 10^{-5}$
9	$3.611163 \cdot 10^{1}$	$2.404579 \cdot 10^{-5}$	$2.424464 \cdot 10^{-5}$
10	$2.511983 \cdot 10^{2}$	$2.404579 \cdot 10^{-5}$	$2.424464 \cdot 10^{-5}$

4.4. Test 3: Stability of Crank–Nicolson scheme

Now let us consider again the problem with nonlocal discrete condition ($v(t) \equiv 0$). The functions $f(x, t)$ and $\varphi(x)$ are chosen so that the function

$$u(x, t) = (\sin(\pi x) + \cos(\pi x) + 2x - 1)\exp(-t)$$

is the exact solution of the problem, i.e.

$$f(x, t) = ((\pi^2 - 1)(\sin(\pi x) + \cos(\pi x)) - (2x - 1))\exp(-t),$$

$$\varphi(x) = (\sin(\pi x) + \cos(\pi x) + 2x - 1)\Big(1 - \sum_{j=1}^{m} \alpha_j \exp(-T_j)\Big).$$

In this numerical experiment, we use $T = 1$, $m = 1$, $\alpha_1 = -10$ and $T_1 = 0.9$.

We solve this problem using Scheme 2 with $h = 1/400$. According to Theorem 3.2 in paper [21], this scheme should be stable if the time step $\tau < \tau_0 = -\log(|\alpha_1|\exp(-\pi^2 T_1))/\pi^4 \approx 0.0675508$. However, from Table 3 we see that Scheme 2 is unstable with $\tau = 1/200 < \tau_0$.

Corollary 4 suggests $\tau_0 = 1/(399\pi) \approx 0.0007977$. In Table 3 we present results obtained with $\tau = 1/2000 < \tau_0$ and we see that Scheme 2 is stable. The revised constraint for the time step size is sufficient but not necessary to ensure the stability. For example, from Table 3 we can see that Scheme 2 is stable with $\tau = 1/1000 > \tau_0$.

4.5. Test 4: Stability of FTCS and Crank–Nicolson schemes

In this example, the test problem has the same solution as in Test 3, but now $T_1 = 0.25$ and $\alpha_1 = -11.75$.

We use $h = 1/20$. Therefore, according to Theorem 1 and Corollaries 3 and 6, the Crank–Nicolson scheme (Scheme 2) is stable whenever $\tau < 0.0000728445$, and for FTCS scheme (Scheme 4) this bound is approximately equal to 0.00137564. Let us say that $\tau = 0.001$. Then our theoretical results state that FTCS (explicit) scheme is stable. From the classical point of view, the Crank–Nicolson (implicit) scheme should be stable too. However, the time step value 0.001 is larger than required in Corollary 3 and, as we can see from Fig. 2, the Crank–Nicolson scheme is unstable. The values of α_1 and $\|\mathbf{S}\|$ act as amplification factors, and $\|\mathbf{S}\|$ is closer to 1 for the Crank–Nicolson scheme than for FTCS scheme. Therefore, the iterative procedure diverges.

Additionally, when $\alpha_1 < -11.7918$, the condition (H) is not satisfied and Scheme 4 does not converge even for very small values of τ.

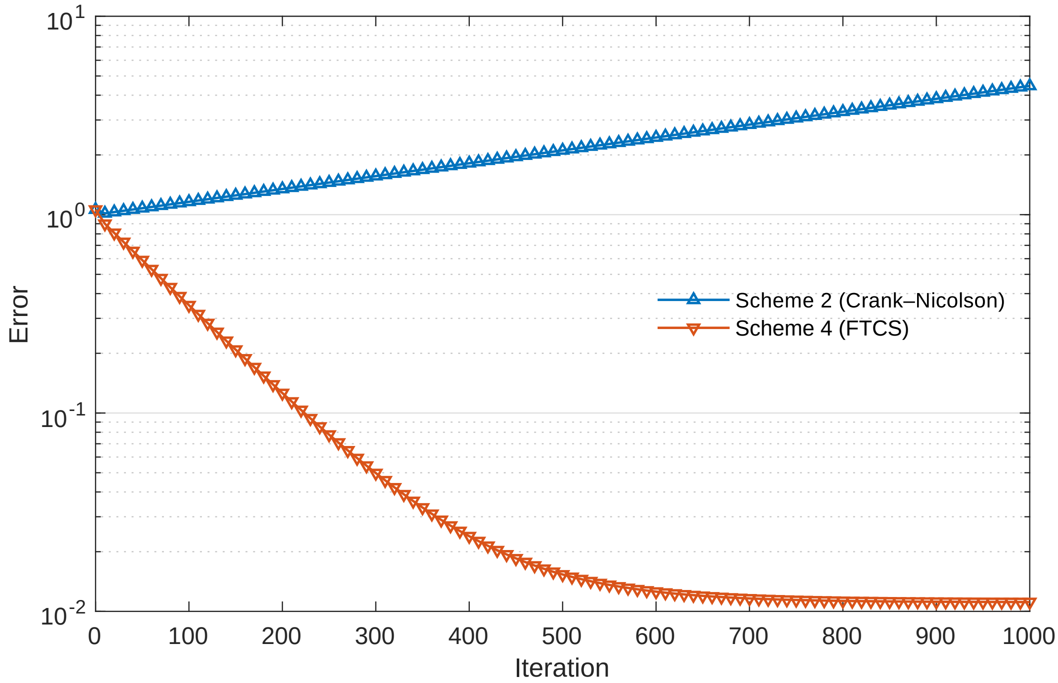


Fig. 2. Maximum norms of the absolute error (E_∞): Test 4, Schemes 2 and 4, $\tau = 1/1000$, $h = 1/20$.

4.6. *Test 5: Nonlinear problem*

In this paper, we focus attention on the finite difference schemes applied to linear problems. For such problems there exist many other numerical techniques and some of them can be even more accurate and efficient. An important advantage of the finite difference technique is that numerical schemes can be easily implemented for nonlinear problems. In such cases, it is necessary to solve a nonlinear system in each iteration.

The convergence and stability of the numerical scheme need to be studied separately for each nonlinear problem. Assuming that the solution $u(x,t)$ (and its discrete counterpart) does not vary too rapidly, such problems also can be analyzed by linearization.

As an example we solve a nonlinear parabolic equation

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = -u^5 + f(x,t), \qquad (x,t) \in \Omega \times (0,T),$$

subject to homogeneous boundary conditions and nonlocal discrete initial condition (3) with $\alpha_1 = 1$, $T_1 = 1$ ($\upsilon(t) \equiv 0$). The functions $f(x,t)$ and $\varphi(x)$ are such that the exact solution is $u(x,t) = \sin(t)\sin(\pi x)$:

$$f(x,t) = (\cos(t) + \pi^2 \sin(t) + \sin(\pi x^4)\sin(t)^5)\sin(\pi x),$$
$$\varphi(x) = -\sin(1)\sin(\pi x).$$

We solve this problem using Scheme 4 with $\tau = h^2/6$. Results are provided in Table 4. We observe the second order accuracy. In this case, two iterations are enough to obtain the prescribed accuracy.

Table 4
Absolute errors ($t = 1$), order of accuracy and the total number of iterations required to achieve the prescribed accuracy: Test 5, Scheme 4, $\tau = h^2/6$.

	Errors			Order	Number of iterations
	$x = 0.25$	$x = 0.5$	$x = 0.75$		
Scheme 4					
$h = 1/20$	$1.03549 \cdot 10^{-3}$	$1.43757 \cdot 10^{-3}$	$1.03549 \cdot 10^{-3}$	–	2
$h = 1/40$	$2.58719 \cdot 10^{-4}$	$3.59293 \cdot 10^{-4}$	$2.58719 \cdot 10^{-4}$	~ 2.0004	2
$h = 1/80$	$6.46702 \cdot 10^{-5}$	$8.9817 \cdot 10^{-5}$	$6.46702 \cdot 10^{-5}$	~ 2.00025	2
$h = 1/160$	$1.6167 \cdot 10^{-5}$	$2.24539 \cdot 10^{-5}$	$1.6167 \cdot 10^{-5}$	~ 2.00017	2

5. Concluding remarks

In this paper, the two-level finite difference schemes for the one-dimensional heat equation with the nonlocal initial condition have been analyzed. We have revised analysis provided in paper [21] and obtained additional restrictions for the time step.

We have demonstrated that the explicit FTCS scheme can be stable while some implicit methods, such as Crank–Nicolson scheme, are unstable. This observation is unexpected from the classical point of view. However, it can be explained by nonlocal nature of initial conditions in the examined problem and iterative procedure for the solution of numerical schemes. Theoretically, we have considered a linear problem only. However, numerically we have checked that the numerical properties of finite difference schemes in a nonlinear case can be similar.

The stability conditions (restrictions for the time step size) we obtained in this paper are related to the minimal and maximal eigenvalues of the tridiagonal symmetric matrix corresponding to the central finite differences. It makes these conditions difficult to apply in practice. In the future, it would be interesting to obtain stability conditions which would allow direct determination of the time step size. Another important direction for the future work is the construction of the numerical schemes for multidimensional PDEs with nonlocal initial conditions and the corresponding extension of the theoretical results.

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