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Approximation of parabolic PDEs with a discontinuous initial condition

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Abstract — We consider a Dirichlet problem for a parabolic partial differential equation with a discontinuous initial condition. The boundary condition at $t = 0$ is assumed to have a discontinuity of the first kind. Due to the singularity of the solution in the neighbourhood of the discontinuity, the usual discretization methods do not yield convergence in the ℓ^∞-norm in the entire domain of definition. Therefore, in order to handle the singularity an adapted scheme is constructed. We use a specially fitted difference operator on a regular rectangular grid. Such a difference scheme converges in the discrete ℓ^∞-norm on the whole uniform grid. For a model problem, numerical experiments with the classical and the specially fitted schemes are compared and discussed.

Keywords. Parabolic PDE, discontinuous boundary condition, finite difference methods, uniform convergence.

Solutions of parabolic boundary value problems with discontinuous initial conditions are not smooth on their domain of definition. Therefore, difficulties arise when these problems are solved by numerical methods. As was shown, e.g. in [6,7] the solutions of difference equations which are constructed on regular rectangular grids using classical schemes do not converge in the ℓ^∞-norm in the neighbourhood of the discontinuity in the boundary condition. Our aim is to construct a scheme which converges in the ℓ^∞-norm throughout the domain of definition.

Different approaches can be used for constructing of such special schemes for problems with non-smooth solutions: (1) methods in which the singularity is split off and represented separately (e.g. by introducing special basis functions in the Finite Element Method); (2) methods that use special, refined meshes in the neighbourhoods of singularities; (3) fitted methods in which the coefficients of the difference equations are adapted to the singularities.

A method combining the second and the third approach was proposed in [6,7]. A second-order one-dimensional parabolic equation with a discontinuous boundary condition was studied; the highest derivative of the equation contained a small parameter $\varepsilon \in (0, 1]$. When $\varepsilon \to 0$, the equation reduces to an equation with only a first-order derivative for the time-variable. A special difference scheme was constructed for this singularly perturbed boundary value problem. This scheme converges uniformly with respect to the small parameter in the ℓ^∞-norm on the whole domain. Outside some neighbourhood of this discontinuity the classical difference scheme was used on a rectangular grid. In the neighbourhood of the discontinuity special parabolic variables as

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$\theta = x/\sqrt{2t}$ and t were applied. Due to these special variables, the singular part of the solution becomes a sufficiently smooth function. Thus, the special scheme [6,7] can be used for a regular parabolic equation with discontinuous initial conditions.

Generally, this approach will be too complex in practice because it involves fitting both the coefficients and the mesh. Therefore in the present paper we propose a new method in which only the coefficients are adapted. We use a uniform rectangular grid and a special difference equation with a fitted coefficient. This coefficient is selected such that the solution of a model problem with a piecewise constant discontinuous initial function is the exact solution of the difference equations. This difference scheme with an adapted coefficient is investigated and the results are compared to those of the classical scheme.

For singularly perturbed elliptic partial differential equations, difference approximations to problems with discontinuous boundary conditions were studied in [8].

1. PROBLEM FORMULATION

On the interval

$$D = \{x \mid -1 < x < 1\} \tag{1.1}$$

we consider the Dirichlet problem for the parabolic equation[†]

$$\begin{aligned} L_{(1.2)}u(x,t) &= f(x,t), \qquad (x,t) \in G \\ u(x,t) &= \varphi(x,t), \qquad (x,t) \in S \end{aligned} \tag{1.2a}$$

where

$$\begin{aligned} G &= D \times (0,T] \\ S = \overline{G} \backslash G &= \{(x,t) \mid x \in [-1,+1],\ t = 0;\ x = \pm 1,\ t \in [0,T]\} \end{aligned} \tag{1.2b}$$

$$L_{(1.2)} \equiv \frac{\partial^2}{\partial x^2} - p(x,t)\frac{\partial}{\partial t} - c(x,t). \tag{1.2c}$$

The coefficients $c(x,t)$, $p(x,t)$ and the right-hand side $f(x,t)$ are sufficiently smooth functions on $\overline{G}$, and the coefficients are positive:

$$c(x,t) \geq 0, \qquad p(x,t) \geq p_0 > 0, \qquad (x,t) \in \overline{G}. \tag{1.3}$$

The boundary function $\varphi(x,t)$ has discontinuities of the first kind on the set S^*. For simplicity, in this paper S^* consists of a single point only:

$$S^* = \{(x,t) \mid x = 0,\ t = 0\}. \tag{1.4}$$

Outside a neighbourhood of S^* the function $\varphi(x,t)$ is sufficiently smooth on S. A piecewise continuous function $v(x,t)$, on $S \backslash S^*$, is redefined at the discontinuity by

$$v(x,t) = \frac{1}{2}\left\{ \lim_{s \to +0} v(x+s,t) + \lim_{s \to -0} v(x+s,t) \right\}, \qquad (x,t) \in S^*. \tag{1.5}$$

These boundary value problems with a discontinuous boundary condition describe, in particular, the temperature in heat transfer problems, when two parts of a material

[†]The subscript number (within brackets) for a symbol denotes the equation where this symbol is defined.

at different temperatures are instantaneously connected. Such problems arise e.g. when analyzing problems of heat conduction in a rolling-mill.

For problem (1.2) we want to find a difference scheme which converges in the discrete ℓ^∞-norm on the whole grid. In order to study the difference scheme, we will make use of a typical model problem on the set $\overline{G} = [-1,1]\times[0,1]$, for the homogeneous heat equation with discontinuous initial condition:

$$L_{(1.6)}u(x,t) = \frac{\partial^2 u(x,t)}{\partial x^2} - \frac{\partial u(x,t)}{\partial t} = 0\,, \qquad (x,t) \in G \tag{1.6a}$$

$$u(x,t) = \varphi(x,t)\,, \qquad (x,t) \in S \tag{1.6b}$$

where $\varphi(x,t)$ is such that the solution of the problem contains either or both smooth and discontinuous components.

2. THE BEHAVIOUR OF THE SOLUTION AND ITS DERIVATIVES

In order to construct special difference schemes for problem (1.2) and study their behaviour, we first need some estimates of the solution and its derivatives. Note that the solution of problem (1.2) is continuous for $t > 0$. The discontinuity appears only at the point $(0,0)$. The derivatives exist and are sufficiently smooth in $\overline{G}$, outside of a neighbourhood of S^*. They only increase, without bound, in the neighbourhood of S^*. Due to the maximum principle, we have for the solution of (1.2) the estimate

$$|u(x,t)| \le M\,, \qquad (x,t) \in \overline{G} \tag{2.1}$$

where

$$M = (p_0)^{-1}T \max_{\overline{G}} |f(x,t)| + \max_{S} |\varphi(x,t)|\,. \tag{2.2}$$

Hereafter by M (or m) we denote a sufficiently large (small) positive constant. In case of difference problems these constants do not depend on the parameters of the grid. The constants do not necessarily represent the same value at different appearances.

We introduce the standard function $w_0(x,t)$, which is discontinuous in S^*,

$$w_0(x,t) = w_0(x,t;p) = \frac{1}{2}v\left(\frac{x}{2}\sqrt{\frac{p}{t}}\right), \qquad (x,t) \in \overline{G}\setminus S^* \tag{2.3}$$

where

$$v(\xi) = \operatorname{erf}(\xi) = \frac{2}{\sqrt{\pi}}\int_0^\xi \exp(-\alpha^2)\,\mathrm{d}\alpha$$

is the error function. For $t = 0$, $(x,t) \in S^*$, the value of $w_0(x,t)$ is defined by continuous extension. The function $w_0(x,t)$ is continuous on the domain $\overline{G}\setminus S^*$ and it is a solution of the constant coefficient equation

$$L_{(2.4)}u(x,t) \equiv \left\{\frac{\partial^2}{\partial x^2} - p\frac{\partial}{\partial t}\right\}u(x,t) = 0\,, \qquad (x,t) \in G\,. \tag{2.4}$$

This function is piecewise constant on S at $t = 0$ and has a discontinuity of the first kind in S^*:

$$[w_0(0,0)] = 1 \tag{2.5}$$

where $[w_0(x,t)]$, $(x,t) \in S^*$ is the jump, defined by

$$[v(x,t)] = \lim_{s \to +0} v(x+s,t) - \lim_{s \to -0} v(x+s,t), \qquad (x,t) \in S^*. \tag{2.6}$$

Suppose that

$$W(x,t) = [\varphi(0,0)]\, w_0(x,t,p(0,0)), \qquad (x,t) \in \overline{G} \setminus S^* \tag{2.7}$$

then the function $W(x,t)$ is continuous on $\overline{G}\setminus S^*$ and has a jump at S^*:

$$[W(x,t)] = [\varphi(x,t)], \qquad (x,t) \in S^*.$$

We write the solution of problem (1.2) as a sum

$$u(x,t) = u_{(2.9)}(x,t) + u_{(2.10)}(x,t), \qquad (x,t) \in \overline{G} \setminus S^* \tag{2.8}$$

where $u_{(2.9)}$ is the solution of the problem

$$\begin{aligned} L_{(1.2)} u(x,t) &= 0, & (x,t) &\in G \\ u(x,t) &= W(x,t), & (x,t) &\in S \end{aligned} \tag{2.9}$$

and $u_{(2.10)}(x,t)$ is the solution of the problem

$$\begin{aligned} L_{(1.2)} u(x,t) &= f(x,t), & (x,t) &\in G \\ u(x,t) &= \varphi(x,t) - W(x,t), & (x,t) &\in S. \end{aligned} \tag{2.10}$$

The function $u_{(2.10)}(x,t)$ is continuous and piecewise smooth on S.

For simplicity we first suppose that $p(x,t) = p(t)$ in the neighbourhood of $x = 0$, function $u_{(2.10)}(x,t)$ is sufficiently smooth on the boundary of G, and a compatibility condition is satisfied at the corner points. Then the following estimates hold

$$\left| \frac{\partial^{k+k_0}}{\partial x^k \partial t^{k_0}} u_{(2.10)}(x,t) \right| \le M, \qquad (x,t) \in \overline{G} \tag{2.11}$$

$$\left| \frac{\partial^{k+k_0}}{\partial x^k \partial t^{k_0}} u_{(2.9)}(x,t) \right| \le M t^{-(k_0 + k/2)}, \qquad (x,t) \in G \setminus S^* \tag{2.12}$$

$$\left| u_{(2.9)}(x,t) - W(x,t) \right| \le M t, \qquad (x,t) \in \overline{G}. \tag{2.13}$$

These bounds are determined by means of *a priori* estimates (see, e.g. [1] and [3]). Thus, for the regular and the singular components of solution (2.8) estimates (2.11)-(2.13) hold.

3. CLASSICAL DIFFERENCE APPROXIMATIONS

3.1. The difference schemes

On the set $\overline{G}$ we introduce the rectangular grid

$$\overline{G}_h = \omega \times \omega_0. \tag{3.1}$$

Here ω and ω_0 are uniform grids on the segments $[-1,1]$ and $[0,T]$ respectively; we denote the space step by h and the time step by τ, so that $x_i = ih$, $i \in \mathbb{Z}$, $x_i \in \overline{D}$, $h = 2/N$, $t^j = j\tau$, $j = 0,1,2,\dots,N_0$, $\tau = T/N_0$, and

$$G_h = G \cap \overline{G}_h, \qquad S_h = S \cap \overline{G}_h, \qquad S_h^* = S^* \cap \overline{G}_h.$$

If the set S_h^* is not empty, the boundary function $\varphi(x,t)$ on the set S_h^* is defined by

$$\varphi(x,t) = \frac{1}{2}\Big\{\lim_{s\to x-0}\varphi(s,t) + \lim_{s\to x+0}\varphi(s,t)\Big\}, \qquad (x,t) \in S_h^*. \tag{3.2}$$

For approximation of equation (1.2) we first use classical difference approximations (see, e.g. [4,5]). In case of an implicit difference scheme we have

$$\begin{aligned} \Lambda_{(3.3)}z(x,t) &= f(x,t), \qquad (x,t) \in G_h \\ z(x,t) &= \varphi(x,t), \qquad (x,t) \in S_h. \end{aligned} \tag{3.3}$$

Where

$$\Lambda_{(3.3)} \equiv \delta_{x\bar{x}} - p(x,t)\delta_{\bar{t}} - c(x,t)$$

with $\delta_{\bar{t}}z(x,t)$ and $\delta_{x\bar{x}}\,z(x,t)$ the usual first and second difference of $z(x,t)$ on the uniform grids ω_0 and ω respectively; the bar denotes the backward difference.

It is well known that the operator $\Lambda_{(3.3)}$ is monotone [5], which implies that the maximum principle holds for difference scheme (3.3).

Remark 3.1. For a restricted time step we also might use the explicit difference scheme

$$\begin{aligned} \Lambda_{(3.4)}z(x,t) &= f_{(3.4)}(x,t), \qquad (x,t) \in G_h \\ z(x,t) &= \varphi(x,t), \qquad (x,t) \in S_h \end{aligned} \tag{3.4}$$

or the weighted difference scheme

$$\begin{aligned} \Lambda_{(3.5)}z(x,t) &= f_{(3.5)}(x,t), \qquad (x,t) \in G_h \\ z(x,t) &= \varphi(x,t), \qquad (x,t) \in S_h \end{aligned} \tag{3.5}$$

where

$$\begin{aligned} f_{(3.4)}(x,t) &= \check{f}(x,t) = f(x,t-\tau) \\ \Lambda_{(3.4)}z(x,t) &\equiv \{\delta_{x\bar{x}} - \check{c}(x,t) - \check{p}(x,t)\delta_t\}\check{z}(x,t) \\ f_{(3.5)}(x,t) &= \beta f(x,t) + (1-\beta)\check{f}(x,t) \\ \Lambda_{(3.5)} &\equiv \beta\Lambda_{(3.3)} + (1-\beta)\Lambda_{(3.4)} \end{aligned}$$

with $\beta \in [0,1]$.

3.2. Results with the classical difference approximation for the model problem

It is obvious that the above classical schemes do not yield ℓ^∞-convergence in the neighbourhood of the singularity in the solution. As an example, we solve model problem (1.6), where

$$\varphi(x,t) = w_0(x,t;1), \qquad (x,t) \in S \tag{3.6}$$

on a uniform grid, by means of scheme (3.3). The true solution of this model problem (1.6), (3.6) is the function $u(x,t) = w_0(x,t;1)$, $(x,t) \in \overline{G} \setminus S^*$.

For different $N = 2/h$ and $N_0 = 1/\tau$ we compute the error

$$E(N,N_0) = \max_{(x,t)\in\overline{G}_h} |z(x,t) - w_0(x,t)|$$

where $z(x,t)$ denotes the numerical solution obtained by the classical difference scheme. The results are shown in Table 1. In this table $E(N,N_0) = \max_{(x,t)\in\overline{G}_h} |e(x,t;N,N_0)|$, is the error for the solution of the model problem (1.6), (3.6); $e(x,t;N,N_0) = z(x,t) - w_0(x,t)$ with $h = 2/N$ and $\tau = 1/N_0$.

Table 1.
Errors $E(N, N_0)$.

N_0	N					
	8	16	32	64	128	256
10	$5.77\cdot10^{-2}$	$6.08\cdot10^{-2}$	$6.16\cdot10^{-2}$	$6.25\cdot10^{-2}$	$6.26\cdot10^{-2}$	$6.26\cdot10^{-2}$
40	$2.48\cdot10^{-2}$	$5.69\cdot10^{-2}$	$6.01\cdot10^{-2}$	$6.10\cdot10^{-2}$	$6.20\cdot10^{-2}$	$6.20\cdot10^{-2}$
160	$2.93\cdot10^{-2}$	$2.47\cdot10^{-2}$	$5.69\cdot10^{-2}$	$6.01\cdot10^{-2}$	$6.10\cdot10^{-2}$	$6.20\cdot10^{-2}$
640	$3.18\cdot10^{-2}$	$2.93\cdot10^{-2}$	$2.47\cdot10^{-2}$	$5.69\cdot10^{-2}$	$6.01\cdot10^{-2}$	$6.10\cdot10^{-2}$
2560	$3.27\cdot10^{-2}$	$3.18\cdot10^{-2}$	$2.93\cdot10^{-2}$	$2.47\cdot10^{-2}$	$5.69\cdot10^{-2}$	$6.01\cdot10^{-2}$
10240	$3.29\cdot10^{-2}$	$3.27\cdot10^{-2}$	$3.18\cdot10^{-2}$	$2.93\cdot10^{-2}$	$2.47\cdot10^{-2}$	$5.69\cdot10^{-2}$

Table 2.
Errors $\hat{E}(\eta)$.

$\eta\times0.025$	2^{-14}	2^{-12}	2^{-10}	2^{-8}	2^{-6}	2^{-4}	2^{-2}	1	2^{2}	2^{4}
$100\times\hat{E}(\eta)$	6.20	6.20	6.10	6.01	5.69	2.47	2.93	3.18	3.27	3.29

Table 3.
Errors $E^{te}(N, N_0)$.

N_0	N					
	8	16	32	64	128	256
10	$3.08\cdot10^{-2}$	$3.39\cdot10^{-2}$	$3.40\cdot10^{-2}$	$3.40\cdot10^{-2}$	$3.40\cdot10^{-2}$	$3.40\cdot10^{-2}$
40	$1.01\cdot10^{-2}$	$9.37\cdot10^{-3}$	$9.28\cdot10^{-3}$	$9.22\cdot10^{-3}$	$9.21\cdot10^{-3}$	$9.21\cdot10^{-3}$
160	$3.77\cdot10^{-3}$	$2.73\cdot10^{-3}$	$2.45\cdot10^{-3}$	$2.38\cdot10^{-3}$	$2.37\cdot10^{-3}$	$2.36\cdot10^{-3}$
640	$2.12\cdot10^{-3}$	$9.97\cdot10^{-4}$	$6.98\cdot10^{-4}$	$6.22\cdot10^{-4}$	$6.02\cdot10^{-4}$	$5.98\cdot10^{-4}$

It is clear that, for a fine mesh, the error is a function of the parameter h^2/τ, and in Table 1 we see that the solution of the classical scheme $z(x,t)$ does not converge to the solution $w_0(x,t)$ for decreasing h or decreasing τ. From Table 1 we also see that errors $E(N, N_0)$ depend on a parameter $\eta = \eta(N, N_0) = h^2/\tau = 4N_0N^{-2}$. The resulting figures for

$$\bar{E}(\eta) = \min_{N,N_0,\eta(N,N_0)=\eta} E(N, N_0)$$

are shown in Table 2. From this table we see that there are no errors less than $2.47 \cdot 10^{-2}$.

Note that $|w_0(x,t)| \leq 0.5$. Then from Table 1 we conclude that we cannot guarantee an error less than 12% for any sufficiently small h and τ. From Table 2 we also see that, with the classical scheme and a uniform grid, there are no errors less than 4.9% *for any small value* of h and τ. This is due to the approximation of the solution in the neighbourhood of the singularity. However, convergence is found in the region $\{G_h,\ t \geq t_0 > 0\}$ that excludes a neighbourhood of $t = 0$. This is observed in Table 3. In this table $E^{t_0}(N, N_0) = \max_{(x,t)\in G_h; t\geq t_0} |e(x,t; N, N_0)|$, with $t_0 = 0.2$; further details as in Table 1.

We can see that on $\{G_h,\ t \geq t_0 > 0\}$ the error vanishes for $N, N_0 \to \infty$.

Hence, if we are only interested in the solution in a region at some distance from the initial singularity at $t = 0$, then the classical scheme can be applied. Thus, we can say that the classical scheme is not suitable if we are interested in the approximate solution of problem (1.2) in the ℓ^∞-norm on the domain $\overline{G} \setminus S^*$.

4. A FITTED DIFFERENCE APPROXIMATION

4.1. An intermediate fitted scheme

On the set $\overline{G}$ we introduce the grid $\overline{G}_h$ as in (3.1). For the approximation of equation (1.2) we use a specially fitted scheme

$$\begin{aligned} \Lambda_{(4.1)} z(x,t) &= f(x,t), \quad && (x,t) \in G_h \\ z(x,t) &= \varphi(x,t), \quad && (x,t) \in S_h \end{aligned} \tag{4.1}$$

where

$$\Lambda_{(4.1)} \equiv \gamma(x,t)\delta_{x\bar{x}} - p(x,t)\delta_{\bar{t}} - c(x,t). \tag{4.2}$$

To show the principle of our technique, the fitting coefficient $\gamma(x,t)$ is first chosen in such a way that the function $w_0(x,t)$, introduced in (2.3), exactly satisfies the difference equation

$$\gamma(x,t)\delta_{x\bar{x}} w_0(x,t;p_1) - p_1\delta_{\bar{t}} w_0(x,t;p_1) \equiv 0$$

where $p_1 = p(0,0)$. Except for a factor, this function $w_0(x,t)$ is the principle part of the singular component of the solution in expression (2.8). This difference equation corresponds to homogeneous equation (1.2a), where the coefficient $p(x,t)$ is 'frozen' at the singularity S^* and where the lower-order coefficient $c(x,t)$ is suppressed. Note that $\delta_{\bar{t}} w_0(x,t;p_1) \neq 0$ and $\delta_{x\bar{x}} w_0(x,t;p_1) \neq 0$ for $(x,t) \in G_h$, $x \neq 0$. It follows immediately that γ is determined by

$$\gamma(x,t) = \frac{p(0,0)\,\delta_{\bar{t}} w_0(x,t;p_1)}{\delta_{x\bar{x}} w_0(x,t;p_1)}, \quad (x,t) \in G_h, \quad x \neq 0. \tag{4.3a}$$

At the nodes S_h^* the function $w_0(x,t)$ is defined by (1.5). Therefore we have, for $(x,t) \in G_h$, $x \neq 0$,

$$\gamma(x,t) = \frac{p(0,0)\,\tau^{-1} \int_{\theta(x,t-\tau)}^{\theta(x,t)} \exp(-\alpha^2)\,d\alpha}{h^{-2}\Big(\int_{\theta(x,t)}^{\theta(x+h,t)} \exp(-\alpha^2)\,d\alpha - \int_{\theta(x-h,t)}^{\theta(x,t)} \exp(-\alpha^2)\,d\alpha \Big)} \tag{4.3b}$$

where

$$\theta(x,t) = \frac{x}{2}\sqrt{\frac{p(0,0)}{t}}\,.$$

For $x = 0$ we set

$$\gamma(x,t) = 1, \qquad (x,t) \in G_h, \qquad x = 0. \tag{4.3c}$$

Difference scheme (4.1) is monotone due to the inequality $\gamma(x,t) > 0$, $(x,t) \in G_h$. Now we study how difference scheme (4.1) approximates the solution of problem (1.2). Due to representation (2.8) we consider the solution of the difference scheme for the solutions of problems (2.9) and (2.10).

Let $v(x,t)$, $(x,t) \in \overline{G}$ be a function satisfying $v \in C^2(G)$, and suppose that $v(x,t)$ is continuous on $\overline{G}\setminus S^*$, and may have a discontinuity of the first kind on S^*. By $z_v(x,t)$, $(x,t) \in \overline{G}_h$, we denote the solution of the difference problem

$$\begin{aligned} \Lambda_{(4.1)} z(x,t) &= f_{(4.4)}(x,t) \equiv L_{(1.2)} v(x,t), \qquad (x,t) \in G_h \\ z(x,t) &= v(x,t), \qquad (x,t) \in S_h \end{aligned} \tag{4.4}$$

where $v(x,t)$ is either $u_{(2.9)}(x,t)$ or $u_{(2.10)}(x,t)$. Let first

$$v(x,t) = u_{(2.10)}(x,t) \tag{4.5}$$

be the part of the solution of problem (1.2) from which we have removed the singular part. Then we estimate the error

$$e_{(4.6)}(x,t) = z_v(x,t) - u_{(2.10)}(x,t), \qquad (x,t) \in \overline{G}_h\,. \tag{4.6}$$

We suppose that $p(x,t) = p(t)$ and estimate (2.11) holds. We use (2.11) and the estimate for $|\gamma(x,t)|$ to obtain

$$|\gamma(x,t)| \le \begin{cases} M(1 + \sqrt{\tau}/h), & t = \tau \\ M, & t > \tau\,. \end{cases}$$

This estimate is derived from (4.3a), where $w_0(x,t;p)$ is given by (2.3). The estimate for the function $e_{(4.6)}(x,t)$ is obtained by applying the maximum principle (as in [2,6]) to the difference problem (4.4), (4.5):

$$|e_{(4.6)}(x,t)| \le M\Big\{\frac{\tau^{3/2}}{h} + t\Big\}, \qquad (x,t) \in \overline{G}_h\,. \tag{4.7}$$

Thus, if $\tau^{3/2}/h$ is small, then the difference between $u_{(2.10)}(x,t)$ and $z_v(x,t)$ is small in the neighbourhood of the line $t = 0$

$$|e_{(4.6)}(x,t)| \le M\Big\{\frac{\tau^{3/2}}{h} + \rho\Big\}, \qquad (x,t) \in \overline{G}_h \tag{4.8}$$

provided that $t \le \rho$, where ρ is an arbitrary number $\rho \in (\tau, T]$.

Further we estimate $e_{(4.6)}(x,t)$ for $t > \rho$. Using estimate (2.11) and an estimate for $|\gamma(x,t) - 1|$ we find the local truncation error. Using (4.3a), (2.3), we find

$$|\gamma(x,t) - 1| \le M\rho^{-2}(h^2 + \tau)$$

for $(x,t) \in \overline{G}_h$ if $t \ge \rho$, and accordingly

$$|\Lambda_{(4.1)} e_{(4.6)}(x,t)| \le M\rho^{-2}(h^2 + \tau) \tag{4.9}$$

for $(x,t) \in \overline{G}_h$ if $t \ge \rho$. Then we apply the maximum principle [5] for $t \ge \rho > 0$ and take into account estimate (4.8) and truncation error (4.9) (at $t \ge \rho$) to obtain the result

$$\begin{aligned} |e_{(4.6)}(x,t)| &= |u_{(2.10)}(x,t) - z_v(x,t)| \\ &\le M\Big\{\max_{x,t\le\rho} |e_{(4.6)}(x,t)| + \max_{x,t\ge\rho} |\Lambda_{(4.1)} e_{(4.6)}(x,t)|\Big\} \\ &\le M\Big\{\rho^{-2}(h^2+\tau) + \frac{\tau^{3/2}}{h} + \rho\Big\}, \qquad (x,t) \in \overline{G}_h, \quad t \ge \rho. \end{aligned}$$

Due to this inequality and (4.8), where $\rho > 0$ is an arbitrary number, we arrive at the estimate

$$|u_{(2.10)}(x,t) - z_v(x,t)| \le M\Big\{(h^2+\tau)^{1/3} + \frac{\tau^{3/2}}{h}\Big\}, \qquad (x,t) \in \overline{G}_h. \tag{4.10}$$

Hence it follows that, under the condition

$$h \ge m\tau^{\nu}, \qquad \nu < 3/2 \tag{4.11}$$

for arbitrary $0 < \nu < 3/2$, convergence of difference problem (4.4) is guaranteed for the smooth solution $v(x,t) = u_{(2.10)}(x,t)$ in expression (2.8)

$$|u_{(2.10)}(x,t) - z_v(x,t)| \le M\big\{(h^2+\tau)^{1/3} + \tau^{3/2-\nu}\big\}, \quad (x,t) \in \overline{G}_h.$$

If, for example,

$$h \ge m\tau^{7/6} \tag{4.12}$$

then we have

$$|u_{(2.10)}(x,t) - z_v(x,t)| \le M(h^2+\tau)^{1/3}, \qquad (x,t) \in \overline{G}_h. \tag{4.13}$$

In a similar way we estimate the function

$$e_{(4.14)}(x,t) = z_v(x,t) - u_{(2.9)}(x,t), \qquad (x,t) \in \overline{G}_h \tag{4.14}$$

where $z_v(x,t)$ is the solution of problem (4.4) with $v(x,t) = u_{(2.9)}(x,t)$. Here, from estimates (2.12) and (2.13) we obtain the estimate

$$|u_{(2.9)}(x,t) - z_v(x,t)| \le M\Big\{(h^2+\tau)^{1/3} + \frac{\tau^{3/2}}{h}\Big\}, \qquad (x,t) \in \overline{G}_h. \tag{4.15}$$

This estimate is derived in the usual way by means of the maximum principle [5], taking into account that $u_{(2.9)}(x,t)$ is the solution of (2.9), where $W(x,t)$ is defined by (2.7), and $w_0(x,t)$ is the solution of problem (2.4) and (2.5). Combining (4.10) and (4.15) we find the result

$$|u_{(1.2)}(x,t) - z_{(4.1)}(x,t)| \le M\left\{(h^2+\tau)^{1/3} + \frac{\tau^{3/2}}{h}\right\}, \qquad (x,t) \in \overline{G}_h. \qquad (4.16)$$

Under condition (4.11) difference scheme (4.1) converges to the solution of problem (1.2),

$$|u_{(1.2)}(x,t) - z_{(4.1)}(x,t)| \le M\left\{(h^2+\tau)^{1/3} + \tau^{3/2-\nu}\right\}, \qquad (x,t) \in \overline{G}_h \qquad (4.17)$$

and under special condition (4.12) we have

$$|u_{(1.2)}(x,t) - z_{(4.1)}(x,t)| \le M(h^2+\tau)^{1/3}, \qquad (x,t) \in \overline{G}_h. \qquad (4.18)$$

Thus, we see that, for $p(x,t) = p(t)$ and under condition (4.11), the solution of difference scheme (4.1) converges to the solution of problem (1.2) in the discrete ℓ^∞-norm on the whole set $\overline{G}_h$, and estimates (4.17) and (4.18) hold under condition (4.11) and (4.12) respectively.

4.2. The final fitted scheme

The function $\gamma(x,t)$ as introduced in (4.3) is not easily used for practical purposes, because the derivatives of $w_0(x,t)$ both in the numerator and in the denominator of (4.3a) decrease exponentially for large $x/\sqrt{t}$ which causes a numerical instability in the computation of $\gamma(x,t)$. Therefore, scheme (4.1) has little practical value and is mainly of theoretical interest. Note, however, that the influence of the special scheme is only required in the neighbourhood of the singularity, where derivatives of the solution of (1.2) are unboundedly large. Therefore we modify $\gamma(x,t)$ so as to be sure that (in a stable way) $\overline{\gamma}(x,t) \to 1$ for increasing $|x|$ or t. This means that the usual classical scheme is practically retained outside a neighbourhood of the discontinuity.

A proper modification of scheme (4.1) is found by replacing the discontinuous function $w_0(x,t)$ in formula (4.3a) by $\tilde{w}(x,t) = w_0(x,t) + v_0(x,t)$, where $v_0(x,t)$ is a smooth function with sign $\delta_{x\bar{x}} v(x,t)$ the same as sign $\delta_{x\bar{x}} w_0(x,t)$. Then

$$\overline{\gamma}(x,t) = \frac{p_1\,\delta_{\bar{t}}\tilde{w}(x,t) + L_{(2.4)}\tilde{w}(x,t)}{\delta_{x\bar{x}}\tilde{w}(x,t)}, \qquad (x,t) \in G_h, \quad x \ne 0. \qquad (4.19)$$

For instance, if $v_0(x,t) = -x^3 - 6(p(0,0))^{-1}xt$, this implies that $\gamma(x,t)$ is replaced by

$$\overline{\gamma}(x,t) = \frac{p(0,0)\,\delta_{\bar{t}} w_0(x,t) - 6x}{\delta_{x\bar{x}} w_0(x,t) - 6x}, \qquad (x,t) \in G_h, \quad x \ne 0 \qquad (4.20)$$

with $\overline{\gamma}(x,t) = 1$, $(x,t) \in G_h$, $x = 0$. In a close neighbourhood of S^* the functions $\overline{\gamma}(x,t)$ and $\gamma(x,t)$ are almost equal [in Fig. 1 we can see the function $\overline{\gamma}(x,t)$ for $p(0,0) = 1$]. The discrete operator (4.2) is accordingly replaced by

$$\Lambda_{(4.22)} \equiv \overline{\gamma}(x,t)\delta_{x\bar{x}} - p(x,t)\delta_{\bar{t}} - c(x,t). \qquad (4.21)$$

Thus we obtain the special difference scheme

$$\begin{aligned} \Lambda_{(4.22)} z_{(4.22)}(x,t) &= f(x,t), \qquad (x,t) \in G_h \\ z_{(4.22)}(x,t) &= \varphi(x,t), \qquad (x,t) \in S_h \end{aligned} \qquad (4.22)$$

which is our new (modified) adapted scheme. The proof of the error estimate

$$|u_{(1.2)}(x,t) - z_{(4.22)}(x,t)| \le M\left\{(h^2+\tau)^{1/3} + \tau^{3/2-\nu}\right\}, \qquad (x,t) \in \overline{G}_h \tag{4.23}$$

under condition (4.11) and the estimate

$$|u_{(1.2)}(x,t) - z_{(4.22)}(x,t)| \le M(h^2+\tau)^{1/3}, \qquad (x,t) \in \overline{G}_h \tag{4.24}$$

under condition (4.12) is similar to that of estimates (4.17), (4.18). Thus, we have the following theorem.

Theorem 4.1. *Assume that (a) $p(x,t) = p(t)$ in the neighbourhood of S^*, and (b) for $k + 2k_0 \le 4$, the estimates (2.11), (2.12) and (2.13) hold for the functions $u_{(2.9)}(x,t)$ and $u_{(2.10)}(x,t)$, which represent the discontinuous and the continuous component of solution u in (2.8). Then, under condition (4.11), the solution of difference scheme (4.22) converges to the solution of problem (1.2) in the discrete ℓ^∞-norm on the whole set $\overline{G}_h$. Under conditions (4.11) or (4.12) respectively, estimates (4.23) or (4.24) hold for the solution of the difference problem.*

Remark 4.1. In schemes (4.1), (3.1), and (4.22), (3.1), the set S^* belongs to the grid $\overline{G}_h$. In the same way as above, we can construct a scheme on $\overline{G}_h$ for which $S^* \not\subset \overline{G}_h$.

If we drop condition (a) of Theorem 4.1 then, for problem (1.2) where $p(x,t)$ and $c(x,t)$ are sufficiently smooth functions, under conditions (4.11) or (4.12) respectively, the estimates

$$|u_{(1.2)}(x,t) - z_{(4.22)}(x,t)| \le M\left\{(h^2+\tau)^{1/5} + \tau^{3/2-\nu}\right\}, \qquad (x,t) \in \overline{G}_h$$

or

$$|u_{(1.2)}(x,t) - z_{(4.22)}(x,t)| \le M(h^2+\tau)^{1/5}, \qquad (x,t) \in \overline{G}_h$$

hold for the solution of the difference problem. This result is obtained by a lengthy and tedious computation along the lines as shown in [6].

5. NUMERICAL RESULTS FOR THE DIFFERENCE SCHEME

5.1. The discretization error for the model problem

To show the effectiveness of the scheme (4.22) we apply it to the solution of model problem (1.6) where $\varphi(x,t)$ is such that the solution of the problem contains both a singular and a regular component

$$u(x,t) = w_0(x,t) - u_{(5.2)}(x,t) \tag{5.1}$$

with

$$u_{(5.2)}(x,t) = (x+0.5)^2 + 2t. \tag{5.2}$$

This implies for the boundary condition

$$\varphi(x,t) = w_0(x,t) - u_{(5.2)}(x,t), \qquad (x,t) \in S. \tag{5.3}$$

For problem (1.6), (5.3) we use the fitted scheme (4.22). Figure 1 shows the fitted function $\overline{\gamma}(x,t)$ for (1.6).

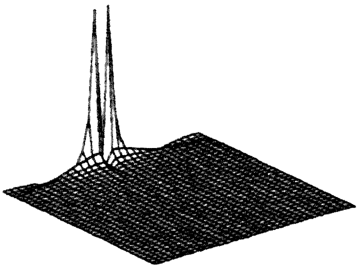

Figure 1. The coefficient $\overline{\gamma}(x,t)$ used in the fitted scheme (4.22), (3.1) as a function of x and t, for problem (1.6), $N = 32$, $N_0 = 40$.

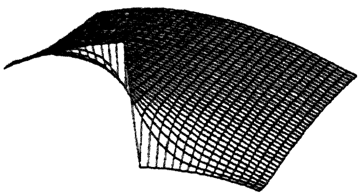

Figure 2. The computed solution obtained with the fitted scheme (4.22), (3.1) for $u(x,t) = u_{(5.1)}(x,t) = w_0(x,t) - u_{(5.2)}(x,t)$, $N = 32$, $N_0 = 40$.

Note that $\overline{\gamma}(x,t)$ is constant (equal to 1) almost everywhere, and only significantly differs from 1 in the neighbourhood of the singularity S^*. The computed solution for problem (1.6) is shown in Figure 2.

We see that this solution has a discontinuity at S^* and is smooth outside a neighbourhood of S^*.

To estimate the errors in the singular solution of the problem (1.6), (5.3) we compute separately the errors for the solution of problem (1.6) with

$$\varphi(x,t) = w_0(x,t), \qquad (x,t) \in S \tag{5.4}$$

and of problem (1.6) with

$$\varphi(x,t) = u_{(5.2)}(x,t), \qquad (x,t) \in S \tag{5.5}$$

where $w_0(x,t)$ and $u_{(5.2)}(x,t)$ are the singular and the regular part of the solution of (1.6), (5.3).

For the error

$$E(N, N_0) = \max_{(x,t)\in\overline{G}_h} |z(x,t) - u(x,t)|$$

experimental results are given in the Tables 4 and 5.

Table 4.
Errors $E(N, N_0)$ in the solution of problem (1.6), (5.4) with $u(x,t) = w_0(x,t;1.0)$. Scheme (4.22), (3.1) is used with $h = 2/N$ and $\tau = 1/N_0$.

N_0	N					
	8	16	32	64	128	256
10	$2.26\cdot10^{-2}$	$1.96\cdot10^{-2}$	$1.89\cdot10^{-2}$	$1.87\cdot10^{-2}$	$1.87\cdot10^{-2}$	$1.87\cdot10^{-2}$
40	$1.27\cdot10^{-2}$	$1.06\cdot10^{-2}$	$1.01\cdot10^{-2}$	$1.00\cdot10^{-2}$	$1.00\cdot10^{-2}$	$1.00\cdot10^{-2}$
160	$7.74\cdot10^{-3}$	$5.30\cdot10^{-3}$	$4.30\cdot10^{-3}$	$4.16\cdot10^{-3}$	$4.08\cdot10^{-3}$	$4.07\cdot10^{-3}$
640	$6.13\cdot10^{-3}$	$3.01\cdot10^{-3}$	$1.80\cdot10^{-3}$	$1.43\cdot10^{-3}$	$1.33\cdot10^{-3}$	$1.31\cdot10^{-3}$
2560	$5.71\cdot10^{-3}$	$2.30\cdot10^{-3}$	$9.47\cdot10^{-4}$	$5.28\cdot10^{-4}$	$4.17\cdot10^{-4}$	$3.88\cdot10^{-4}$
10240	$5.61\cdot10^{-3}$	$2.11\cdot10^{-3}$	$7.00\cdot10^{-4}$	$2.64\cdot10^{-4}$	$1.44\cdot10^{-4}$	$1.12\cdot10^{-4}$

Table 5.
Errors $E(N, N_0)$ in the solution of problem (1.6), (5.5) with $u(x,t) = u_{(5.2)}(x,t;1.0)$. Scheme (4.22), (3.1) is used with $h = 2/N$ and $\tau = 1/N_0$.

N_0	N					
	8	16	32	64	128	256
10	$5.10\cdot10^{-2}$	$8.72\cdot10^{-2}$	$1.16\cdot10^{-1}$	$1.36\cdot10^{-1}$	$1.47\cdot10^{-1}$	$1.53\cdot10^{-1}$
40	$1.46\cdot10^{-2}$	$2.27\cdot10^{-2}$	$3.15\cdot10^{-2}$	$3.89\cdot10^{-2}$	$4.50\cdot10^{-2}$	$4.87\cdot10^{-2}$
160	$7.19\cdot10^{-3}$	$5.87\cdot10^{-3}$	$7.00\cdot10^{-3}$	$8.44\cdot10^{-3}$	$9.83\cdot10^{-3}$	$1.10\cdot10^{-2}$
640	$7.32\cdot10^{-3}$	$4.05\cdot10^{-3}$	$2.74\cdot10^{-3}$	$2.22\cdot10^{-3}$	$2.07\cdot10^{-3}$	$2.32\cdot10^{-3}$
2560	$7.44\cdot10^{-3}$	$3.17\cdot10^{-3}$	$1.64\cdot10^{-3}$	$1.03\cdot10^{-3}$	$8.52\cdot10^{-4}$	$8.73\cdot10^{-4}$

From Tables 4 and 5 we see that the solution of difference scheme (4.22), (3.1) approximates both the singular and the regular parts of the solution of problem (1.6). For both parts of the solution the relative error is guaranteed to be not larger than 1% if we take $N \geq 8$ and $N_0 \geq 160$.

Results obtained with scheme (4.22) are also shown in Figure 3. The results obtained with classical scheme (3.3) are shown in Figure 4.

We observe that the error $e(x,t;N,N_0) = z(x,t) - u_{(5.1)}(x,t)$, $(x,t) \in G_h$, is mainly localized in the neighbourhood of S^* and that the error for the classical scheme is much larger than that for the fitted scheme.

Thus, we see that special fitted scheme (4.22) converges for both the singular and the smooth parts (and hence on the whole solution) of model problem (1.6), (5.3), in the discrete ℓ^∞-norm on the whole set $\overline{G}_h$.

5.2. The experimental generalized order of convergence

To realize the value of the difference scheme (4.22) in practice, we determine its order of convergence. To do so, we compute the generalized order of convergence for the error. We say that a difference scheme has a *generalized order* of convergence ν if

$$E(N, N_0) = \max_{(x,t)\in\overline{G}_h} |z(x,t) - u(x,t)| \leq M(h^2 + \tau)^\nu .$$

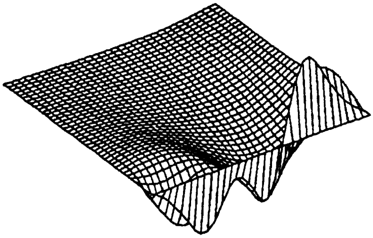

Figure 3. The discretization error for fitted scheme (4.22), (3.1) applied to the same problem as in Figure 2. The maximum error is 0.05545.

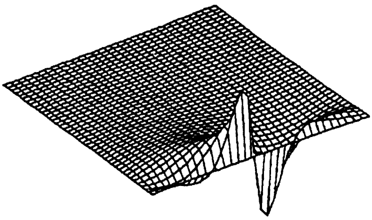

Figure 4. The discretization error for classical scheme (3.3), (3.1) applied to the same problem as in Figure 2. The maximum error is 0.3007.

Here we denote the error by $E(N, N_0)$, where $N = 2/h$ and $N_0 = 1/\tau$. We introduce the *experimental generalized order* of convergence by

$$\overline{\nu} = \min_{N,N_0} \overline{\nu}(N, N_0)$$

where

$$\overline{\nu}(N, N_0) = \{\ln E(N, N_0) - \ln E(2N, 4N_0)\} / \ln 4$$

is the experimental generalized local order of convergence at the point (N, N_0).

Numerical results for the singular and the smooth part of the solution of problem (1.6), (5.3) are shown for the solution $u(x,t) = w_0(x,t)$ in Table 6 and for the solution $u(x,t) = u_{(5.2)}(x,t)$ in Table 7.

In Table 6 it is seen that for the singular part of the solution of problem (1.6), (5.3) the experimental generalized order of convergence is not less than $\overline{\nu} = 0.45$. For the smooth part of the solution of problem (1.6), (5.3) we find (Table 7) the experimental generalized order of convergence to be not less than $\overline{\nu} = 0.41$.

Hence, for our model problem (1.6), (5.3) the value $\bar{\nu}$, which is the experimental generalized order of convergence for our fitted difference scheme (4.22), is not less than 0.4. This order is in agreement with the theoretical lower bound value found in (4.18).

6. CONCLUSION

For the Dirichlet boundary value problem (1.2) for a parabolic equation with variable coefficients and with a discontinuous initial condition we have constructed the adapted scheme (4.22) on a uniform grid (3.1), which converges in the discrete ℓ^∞-norm on the whole grid $\overline{G}_h$.

Both in theory and in practice we have shown that the classical scheme does not converge in the ℓ^∞-norm on all of $\overline{G}_h$. For a model problem (the heat equation with a discontinuous initial condition) in the discrete ℓ^∞-norm no error less than 5% could be found and no error less than 12% could be guaranteed for an arbitrarily small τ and h.

For the same model problem, the special, fitted difference scheme (4.22) converges in the discrete ℓ^∞-norm on the whole grid $\overline{G}_h$, and the experiment shows the generalized order of convergence to be not less than 0.4 (see Tables 6 and 7). This is in agreement with the theory. Moreover, the numerical results show that the special difference scheme (4.22) is efficient indeed: for a typical problem, for $N_0 \geq 160$ and $N \geq 8$, the error is guaranteed to be not larger that 1%, for both the regular and the singular part of the solution.

Table 6.
Experimental generalized local order of convergence $\bar{\nu}(N, N_0)$.
Data derived from the errors as found in Table 4.

N_0	N				
	8	16	32	64	128
10	$5.44 \cdot 10^{-1}$	$4.80 \cdot 10^{-1}$	$4.54 \cdot 10^{-1}$	$4.50 \cdot 10^{-1}$	$4.50 \cdot 10^{-1}$
40	$6.31 \cdot 10^{-1}$	$6.53 \cdot 10^{-1}$	$6.40 \cdot 10^{-1}$	$6.50 \cdot 10^{-1}$	$6.51 \cdot 10^{-1}$
160	$6.81 \cdot 10^{-1}$	$7.82 \cdot 10^{-1}$	$7.92 \cdot 10^{-1}$	$8.18 \cdot 10^{-1}$	$8.18 \cdot 10^{-1}$
640	$7.08 \cdot 10^{-1}$	$8.34 \cdot 10^{-1}$	$8.82 \cdot 10^{-1}$	$8.91 \cdot 10^{-1}$	$8.92 \cdot 10^{-1}$
2560	$7.15 \cdot 10^{-1}$	$8.58 \cdot 10^{-1}$	$9.22 \cdot 10^{-1}$	$9.38 \cdot 10^{-1}$	$9.45 \cdot 10^{-1}$

Table 7.
Experimental generalized local order of convergence $\bar{\nu}(N, N_0)$.
Data derived from the errors as found in Table 5.

N_0	N				
	8	16	32	64	128
10	$5.830 \cdot 10^{-1}$	$7.357 \cdot 10^{-1}$	$7.888 \cdot 10^{-1}$	$7.953 \cdot 10^{-1}$	$7.979 \cdot 10^{-1}$
40	$6.562 \cdot 10^{-1}$	$8.501 \cdot 10^{-1}$	$9.489 \cdot 10^{-1}$	$9.923 \cdot 10^{-1}$	1.016
160	$4.130 \cdot 10^{-1}$	$5.509 \cdot 10^{-1}$	$8.276 \cdot 10^{-1}$	1.012	1.0409
640	$6.035 \cdot 10^{-1}$	$6.518 \cdot 10^{-1}$	$7.017 \cdot 10^{-1}$	$6.914 \cdot 10^{-1}$	$6.250 \cdot 10^{-1}$

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