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A Direct Numerical Procedure for the Cauchy Problem for the Heat Equation*

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For the Cauchy problem, $u_t = u_{xx}$, $0 < x < 1$, $0 < t \leqslant T$, $u(0, t) = f(t)$, $0 < t \leqslant T$, $u_x(0, t) = g(t)$, $0 < t \leqslant T$, a direct numerical procedure involving the elementary solution of $v_t = v_{xx}$, $0 < x$, $0 < t \leqslant T$, $v_x(0, t) = g(t)$, $0 < t \leqslant T$, $v(x, 0) = 0$, $0 < x$ and a Taylor's series computed from $f(t) - v(0, t)$ is studied. Continuous dependence better than any power of logarithmic is obtained. Some numerical results are presented.

1. INTRODUCTION

In this paper, we present a direct numerical procedure for approximating the solution $u = u(x, t)$ of the problem

$$\begin{aligned}
&\text{(a)}\quad u_t = u_{xx}, && 0 < x < 1, \quad 0 < t \leqslant T,\\
&\text{(b)}\quad u(0, t) = f(t), && 0 < t \leqslant T, \qquad\qquad (1.1)\\
&\text{(c)}\quad u_x(0, t) = g(t), && 0 < t \leqslant T,
\end{aligned}$$

where the data f and g are known only approximately as f^* and g^* such that

$$\text{(a)}\qquad \|f - f^*\| < \epsilon,$$

and $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ (1.2)

$$\text{(b)}\qquad \|g - g^*\| < \epsilon,$$

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where $\epsilon > 0$ and for any function $h = h(t)$

$$\| h \| = \sup_{0<t<T} | h(t) | .$$

Since the Cauchy problem (1.1) is not well posed in the sense of Hadamard [1, 3, 10], we add the stabilizing assumption that there exists a constant $M > 0$ such that for $0 < x < 1$, $0 < t \leqslant T$,

$$| u(x, t) | < M. \tag{1.3}$$

Note that we have already assumed that u exists as a classical solution of (1.1). We shall add additional assumptions upon f and g later as needed.

In [10], Carlo Pucci studied the Cauchy problem for a linear parabolic partial differential equation. Under the additional assumption of positivity of the solutions, he demonstrated the continuous dependence of the solution upon the bounds for the solution and its first derivatives at a certain portion of the boundary. No estimate of the degree of continuity was obtained. In [6], Ginsberg considered the Cauchy problem (1.1)–(1.3) and obtained Hölder continuous dependence upon the data. His numerical procedure for $g = 0$ involved expanding f in a Fourier series, thus requiring several numerical quadratures. In [1], one of the present authors presented explicit estimates for Hölder continuity of (1.1)–(1.3) and reduced the problem of numerical approximation to that of the mathematical programming techniques of Douglas [5] for solving Volterra integral equations of the first kind. In [3], Cannon and Douglas considered the Cauchy problem for the heat equation with the data specified on a curve $x = s(t)$. Hölder continuous dependence was derived for solutions satisfying an a priori bound, applications to the Inverse Stefan Problem were given, and a mathematical programming method was presented for its numerical solution.

In the works cited above a great computing effort produces results which are essentially worthless in the neighborhood of any boundary on which no data are specified. Consequently, it is of interest to consider a direct method which has a reduced computing effort and which hopefully produces results reasonably far away from the data-bearing portion of the boundary. The direct numerical procedure studied in this paper is that of approximating u via the solution of the second boundary-initial value problem for the quarter plane:

$$v = \int_0^t g(\tau) \, (4\pi(t - \tau))^{-1/2} \exp\{-x^2(4(t - \tau))^{-1}\} \, d\tau \tag{1.4}$$

and a Taylor's series in x computed from $f - v(0, t)$. Using this approach, we achieve results in the interval $0 \leqslant x < 1/\sqrt{2}$, or approximately 70% of the interval under consideration. In the next section, we develop preliminary estimates to be used later in this paper. Section 3 contains a development of the direct numerical method, together with an explicit estimate of the continuous dependence upon the data. The dependence lies somewhere between any power of the logarithmic estimate and any Hölder estimate. Some basic computational aspects and problems are discussed in Section 4.

2. Preliminary Estimates

From the linearity of the heat equation it follows that the solution u of (1.1)–(1.3) can be written as

$$u = v + w, \tag{2.1}$$

where v satisfies

$$\begin{array}{lll} \text{(a)} & v_t = v_{xx}\,, & 0 < x, \quad 0 < t \leqslant T, \\ \text{(b)} & v_x(0, t) = g(t), & 0 < t \leqslant T, \\ \text{(c)} & v(x, 0) = 0, & 0 < x, \end{array} \tag{2.2}$$

and w satisfies

$$\begin{array}{llll} \text{(a)} & w_t = w_{xx}\,, & 0 < x < 1, & 0 < t \leqslant T, \\ \text{(b)} & w(0, t) = f(t) - v(0, t), & & 0 < t \leqslant T, \\ \text{(c)} & w_x(0, t) = 0, & & 0 < t \leqslant T, \\ \text{(d)} & |\, w(x, 0)| < M, & & 0 < x < 1. \end{array} \tag{2.3}$$

Since the bounded solution of (2.2) is given by

$$v(x, t) = \int_0^t g(\tau)\, (4\pi(t-\tau))^{1/2} \exp \left\{ - \frac{x^2}{4(t-\tau)} \right\} d\tau, \tag{2.4}$$

it follows from elementary estimates [1] that

$$|\, v(x, t)| \leqslant M_1 \, \| g \| \,, \tag{2.5}$$

where

$$M_1 = \pi^{-1/2} T^{1/2} + 2^{-1}. \tag{2.6}$$

Now, by constructing an even extension of w, we see that

$$\begin{array}{lll}
\text{(a)} & w_t = w_{xx}, \quad -1 < x < 1, & 0 < t \leqslant T, \\
\text{(b)} & w(0, t) = f(t) - v(0, t), & 0 < t \leqslant T, \\
\text{(c)} & w_x(0, t) = 0, & 0 < t \leqslant T, \\
\text{(d)} & |w(x, 0)| < M, & -1 < x < 1, \\
\text{(e)} & |w(-1, t)| < M + M_1 \|g\|, & 0 < t \leqslant T, \\
\text{(f)} & |w(1, t)| < M + M_1 \|g\|, & 0 < t \leqslant T.
\end{array} \tag{2.7}$$

Hence, it follows from (2.7) (see [1, 2]) that w can be extended to an analytic function of the complex variable $z = x + iy$ in the domains

$$G_\mu = \{z\colon -1 < x < 1, |y| < \mu(x+1), |y| < \mu(1-x)\} \tag{2.8}$$

for any μ satisfying $0 < \mu < 1$. Employing the elementary estimates given in [1, 2], we see that for $0 < \delta \leqslant t \leqslant T$ and $z \in G_\mu$,

$$|w(z, t)| \leqslant M_2, \tag{2.9}$$

where

$$\begin{aligned} M_2 &= M_2(\delta, \mu) \\ &= M(\pi\delta)^{-1/2} \exp\{(4\delta)^{-1}\} \left(1 + \left(\frac{1+\mu}{1-\mu}\right)^{1/2}\right) + (M + M_1 \|g\|) \left(\frac{1+\mu}{1-\mu}\right)^{1/2}. \end{aligned} \tag{2.10}$$

There is a $\mu_0 > 0$ such that the disc $|z| < \frac{2}{3}$ is contained in G_{μ_0}. As w can be represented as a power series in that disc, estimates for the coefficients of that power series can be obtained from the Cauchy–Riemann Integral Formula. Thus,

$$\frac{1}{n!} \left| \frac{\partial^n w}{\partial x^n}(0, t) \right| \leqslant M_2 \left(\frac{3}{2}\right)^n, \qquad n = 1, 2, 3,... \tag{2.11}$$

for $0 < \delta \leqslant t \leqslant T$.

3. Numerical Approximation

Let $v^{**}(x, t)$ denote a numerical approximation of the quadrature

$$v^*(x, t) = \int_0^t g^*(\tau)\, (4\pi(t-\tau))^{-1/2} \exp\left\{\frac{-x^2}{4(t-\tau)}\right\} d\tau, \tag{3.1}$$

and let

$$w_n^{**}(x, t) = w^{**}(0, t) + \sum_{i=1}^{[(n-1)/2]} \frac{\Delta_i w^{**}(0, t)}{h_i^i} \frac{x^{2i}}{(2i)!}, \tag{3.2}$$

where

$$w^{**}(0, t) = \{f^*(t) - v^{**}(0, t)\} \tag{3.3}$$

and $\Delta_i w^{**}(0, t)/h_i^i$ denotes a standard forward difference approximation to $(\partial^i w/\partial t^i)(0, t)$ [7, 8, 9] with mesh size h_i. As our approximation to u, we set

$$u_n^{**}(x, t) = v^{**}(x, t) + w_n^{**}(x, t). \tag{3.4}$$

In the following paragraphs, we shall describe how one should choose the h_i and the n in order to achieve good accuracy. These choices will arise from a discussion of the error in the approximation to u.

First, set

$$z = v - v^*. \tag{3.5}$$

Then, from (1.2) and (2.5), it follows that

$$|z(x, t)| \leqslant M_1 \epsilon \tag{3.6}$$

for all $0 < x < 1$ and $0 < t \leqslant T$. Clearly, the quadrature approximation can be made as accurately as desired. Hence, there exists a constant M_3 such that

$$|v(x, t) - v^{**}(x, t)| \leqslant M_3 \epsilon. \tag{3.7}$$

Next, we need to estimate the tail of the power series representation for w. Since $w_x(0, t) = 0$ implies that every odd x-derivative of w vanishes at $x = 0$, it follows that for n odd

$$\sum_{i=n+1}^{\infty} \frac{\partial^i w}{\partial x^i}(0, t) \frac{x^i}{(i)!} = \sum_{i=(n+1)/2}^{\infty} \frac{\partial^{2i} w}{\partial x^{2i}}(0, t) \frac{x^{2i}}{(2i)!}, \tag{3.8}$$

whence it follows from (2.11) that for $|x| \leqslant \frac{1}{2}$,

$$\left| \sum_{i=(n+1)/2}^{\infty} \frac{\partial^{2i} w}{\partial x^{2i}}(0, t) \frac{x^{2i}}{(2i)!} \right| \leqslant M_4 \left(\frac{3}{2} x\right)^{n+1}, \tag{3.9}$$

where

$$M_4 = \tfrac{16}{7} M_2. \tag{3.10}$$

Now, we need to estimate the first n terms in the power series for w. Recalling (3.3), it follows from (1.2) and (3.7) that

$$\begin{aligned} |w(0,t) - w^{**}(0,t)| &\leqslant |(f(0,t) - v(0,t)) - (f^*(0,t) - v^{**}(0,t))| \\ &\leqslant \|f - f^*\| + \sup_{\substack{0<t\leqslant T \\ 0<x<1}} |v(x,t) - v^{**}(x,t)| \\ &\leqslant \epsilon + M_3\epsilon = M_5\epsilon. \end{aligned} \tag{3.11}$$

For each $i = 1, 2, \ldots, (n - 1)/2$, we see that

$$\begin{aligned} &\left| \frac{\partial^{2i} w}{\partial x^{2i}}(0,t) - \frac{\Delta_i w^{**}(0,t)}{h_i^{\,i}} \right| \\ &\quad\leqslant \left| \frac{\partial^{2i} w}{\partial x^{2i}}(0,t) - \frac{\Delta_i w(0,t)}{h_i^{\,i}} \right| + |\Delta_i w(0,t) - \Delta_i w^{**}(0,t)| \frac{1}{h_i^{\,i}}, \end{aligned} \tag{3.12}$$

where $\Delta_i w(0,t)/h_i^{\,i}$ is the finite difference approximation of $(\partial^i w/\partial t^i)(0,t)$. From [9, p. 158] and (2.11) we see that for $i = 1, 2, \ldots, (n - 1)/2$,

$$\begin{aligned} \left| \frac{\partial^{2i} w}{\partial x^{2i}}(0,t) - \frac{\Delta_i w(0,t)}{h_i^{\,i}} \right| &= \left| \frac{\partial^{i} w}{\partial t^{i}}(0,t) - \frac{\Delta_i w(0,t)}{h_i^{\,i}} \right| \\ &\leqslant \sup_{\delta\leqslant\tau\leqslant T} \left| \frac{\partial^{i+1} w}{\partial t^{i+1}}(0,\tau) \right| \frac{1}{2} i h_i \\ &\leqslant \sup_{\delta\leqslant\tau\leqslant T} \left| \frac{\partial^{2i+2} w}{\partial x^{2i+2}}(0,\tau) \right| \frac{1}{2} i h_i \\ &\leqslant \frac{M_2}{2}(2i+2)! \left(\frac{3}{2}\right)^{2i+2} i h_i\,. \end{aligned} \tag{3.13}$$

Then, using [7, p. 92] and (3.11), we have

$$\begin{aligned} &|\Delta_i w(0,t) - \Delta_i w^{**}(0,t)| \frac{1}{h_i^{\,i}} \\ &\quad= i! \sum_{s=0}^{i} \frac{w(0,t_s) - w^{**}(0,t_s)}{(t_s - t_0)\cdots(t_s - t_{s-1})(t_s - t_{s+1})\cdots(t_s - t_i)} \\ &\quad\leqslant \frac{i!}{h_i^{\,i}} \sum_{s=1}^{i} |w(0,t_s) - w^{**}(0,t_s)| \\ &\quad\leqslant \frac{M_5(i+1)!\,\epsilon}{h_i^{\,i}}. \end{aligned} \tag{3.14}$$

Combining (3.12)–(3.14) we see that for each $i = 1, 2, \ldots, (n-1)/2$,

$$\left| \frac{\partial^{2i} w}{\partial x^{2i}}(0, t) - \frac{\Delta_i w^{**}(0, t)}{h_i^{\,i}} \right| \leqslant \frac{M_2}{2}(2i+2)! \left(\frac{3}{2}\right)^{2i+2} i h_i + \frac{M_5 (i+1)!\, \epsilon}{h_i^{\,i}}. \tag{3.15}$$

Now for each $i = 1, 2, \ldots, (n-1)/2$, we want to choose an optimal h_i. Differentiating the right-hand side of (3.15) with respect to h_i and setting the result equal to zero, we obtain as an optimal choice for h_i,

$$h_i = \left[\frac{2M_5(i+1)!\, \epsilon}{M_2(2i+2)!\, (\frac{3}{2})^{2i+2}}\right]^{1/(i+1)}. \tag{3.16}$$

With this choice of h_i, we obtain from (3.15)

$$\begin{aligned} &\left| \frac{\partial^{2i} w}{\partial x^{2i}}(0, t) - \frac{\Delta_i w^{**}(0, t)}{h_i^{\,i}} \right| \\ &\quad \leqslant M_2(2i+2)! \left(\frac{3}{2}\right)^{2i+2} i \left[\frac{2M_5(i+1)!\, \epsilon}{M_2(2i+2)!\, (\frac{3}{2})^{2i+2}}\right]^{1/(i+1)} \\ &\quad \leqslant i M_2 (2i+2)!\, (\tfrac{3}{2})^{2i+2} [M_6 \epsilon]^{1/(i+1)}, \end{aligned} \tag{3.17}$$

where

$$M_6 = 2M_5/M_2. \tag{3.18}$$

We can now estimate the error between u and u^{**}. Letting w_n be the first n terms of w, it follows from (3.11) and (3.17) that for all $0 \leqslant x \leqslant \frac{1}{2}$, $\delta \leqslant t \leqslant T$,

$$\begin{aligned} &| w_n(x, t) - w_n^{**}(x, t)| \\ &\quad \leqslant | w(0, t) - w^{**}(0, t)| + \sum_{i=1}^{(n-1)/2} \left| \frac{\partial^{2i} w}{\partial x^{2i}}(0, t) - \frac{\Delta_i w^{**}(0, t)}{h_i^{\,i}} \right| \frac{x^{2i}}{(2i)!} \\ &\quad \leqslant M_5 \epsilon + (n+1)^3 \sum_{i=1}^{(n-1)/2} M_7 (\tfrac{9}{4} x^2)^i\, \epsilon^{1/(i+1)} \\ &\quad \leqslant M_5 \epsilon + M_9 (n+1)^3\, \epsilon^{1/(n+1)}. \end{aligned} \tag{3.19}$$

Now, using the triangle inequality along with (3.7), (3.9), and (3.19), we obtain

$$\begin{aligned} | u(x, t) - u^{**}(x, t)| &= | v(x, t) + w(x, t) - v^{**}(x, t) - w_n^{**}(x, t)| \\ &\leqslant | v(x, t) - v^{**}(x, t)| + | w_n(x, t) - w_n^{**}(x, t)| \\ &\quad + \left| \sum_{i=(n+1)/2}^{\infty} \frac{\partial^{2i} w}{\partial x^{2i}}(0, t) \frac{x^{2i}}{(2i)!} \right| \\ &\leqslant M_{10}(n+1)^3\, \epsilon^{1/(n+1)} + M_4 (\tfrac{3}{2} x)^{n+1} \end{aligned} \tag{3.20}$$

for all $0 \leqslant x \leqslant \frac{1}{2}$, $\delta \leqslant t \leqslant T$. We see that if we choose

$$n + 1 = \frac{\log \epsilon^{-1}}{\log(\frac{3}{2}x)^{-1}}, \tag{3.21}$$

in (3.20), then

$$\begin{aligned} &| u(x, t) - u^{**}(x, t)| \\ &\quad \leqslant M_{10} \left\{ \frac{\log \epsilon^{-1}}{\log(\frac{3}{2}x)^{-1}} \right\}^{3/2} \exp \left[- \left(\log \epsilon^{-1} \log \left(\frac{3}{2} x \right)^{-1} \right)^{1/2} \right] \\ &\quad\quad + M_4 \exp[-(\log \epsilon^{-1} \log(\tfrac{3}{2}x)^{-1})^{1/2}]. \end{aligned} \tag{3.22}$$

Using the simple estimate that

$$e^{-x} < n!/x^n, \tag{3.23}$$

we can see that the estimate (3.22) gives *better than* logarithmic continuity for the approximation of u by u^{**}. The discussion concerning (3.21) shows that the choice for the truncation should be

$$n = \left[\!\left[\left\{ \frac{\log \epsilon^{-1}}{\log(\frac{3}{2}x)^{-1}} \right\}^{1/2} \right]\!\right] - 1, \tag{3.24}$$

where $[\![\cdot]\!]$ is the standard greatest integer function.

4. Computational Aspects

Recalling (3.1), we note that for $x > 0$ the kernel is not singular. Hence, any standard quadrature scheme can be used to approximate $v^*(x, t)$. However, $v^*(0, t)$ results from a weakly singular kernel convolved with g^*. For this particular kernel, Cannon, Hampton and Strauss [4] have devised a quadrature scheme based upon linear interpolation of g^* between mesh points and the analytic quadrature of the kernel convolved with the resulting linear functions over the intervals between consecutive mesh points. It has been recommended to the authors that one should not use the same mesh points as those for the finite differences and that for complicated g a better interpolation will be needed [11].

We noted in Section 3 that the h_i, $i = 1, 2,..., (n - 1)/2$, should optimally be chosen according to (3.16). We also note that the h_i will determine the locations and spacing of the data points for (1.2). We can reduce the number of different h_i needed in our computations by considering the following table which gives h_i as a function of $2M_5\epsilon/M_2$.

TABLE I

$2M_5\epsilon/M_2$

i	0.1	0.01	0.001	0.0001
1	0.0406	0.0128	0.0041	0.0013
2	0.0418	0.0194	0.0090	0.0042
3	0.0390	0.0220	0.0123	0.0070
4	0.0356	0.0225	0.0142	0.0090
5	0.0324	0.0221	0.0150	0.0103
6	0.0296	0.0213	0.0153	0.0110
7	0.0271	0.0203	0.0153	0.0114
8	0.0250	0.0194	0.0150	0.0116
9	0.0232	0.0184	0.0146	0.0116
10	0.0216	0.0175	0.0142	0.0115

We conclude that three different choices of h_i will suffice for each choice of $2M_5\epsilon/M_2$ if we consider $n \leqslant 10$ (20 terms in our power series). In particular for $2M_5\epsilon/M_2 = 0.0001$, letting $h_1 = .001$, $h_2 = h_3 = .005$, and $h_4 = h_5 = \cdots = h_{10} = .01$ will suffice. We shall use this choice in the computation of some of the numerical results in Section 5.

5. Numerical Results

In order to test our numerical procedure we choose to use as our example the problem of finding V such that

$$\begin{array}{lll}
\text{(a)} & V_t = V_{xx}, & 0 < x < 1, \quad 0 < t, \\
\text{(b)} & V(1, t) = 1, & 0 < t, \\
\text{(c)} & V(x, 0) = 0, & 0 < x < 1.
\end{array} \tag{5.1}$$

We see that the function

$$V(x, t) = 1 + 2 \sum_{n=0}^{\infty} \exp\{-(2n+1)^2 \pi^2 t/4\} F(n, x) \tag{5.2}$$

where

$$F(n, x) = \left[\frac{(-1)^{n+1}\, 2}{(2n+1)\,\pi}\right] \cos \left\{\frac{(2n+1)\,\pi x}{2}\right\} \tag{5.3}$$

is a solution to the boundary value problem defined by (5.1) satisfying, in addition, the condition

$$V_x(0, t) = 0. \tag{5.4}$$

TABLE II

	.1% Data Error		Truncation $n = 2$	
X	$V(x, t)$	$u^{**}(x, t)$	$\lvert V(x, t) - u^{**}(x, t)\rvert$	% Error
.10	0.004931	0.004923	0.000008	0.1592
.20	0.011560	0.011478	0.000082	0.7087
.30	0.026896	0.026332	0.000564	2.0976
.40	0.057789	0.055378	0.002411	4.1726
.50	0.113848	0.106866	0.006982	6.1325
.60	0.205904	0.191406	0.014498	7.0413
.70	0.342782	0.321961	0.020821	6.0741
.80	0.527089	0.513855	0.013234	2.5108
.90	0.751830	0.784767	0.032937	4.3810
1.00	1.000000	1.154736	0.154736	15.4736

TABLE III

	.1% Data Error		Truncation $n = 8$	
X	$V(x, t)$	$u^{**}(x, t)$	$\lvert V(x, t) - u^{**}(x, t)\rvert$	% Error
.10	0.004931	0.004924	0.000007	0.1475
.20	0.011560	0.011513	0.000047	0.4074
.30	0.026896	0.026686	0.000210	0.7806
.40	0.057789	0.057031	0.000758	1.3110
.50	0.113848	0.111541	0.002307	2.0266
.60	0.205904	0.199647	0.006257	3.0387
.70	0.342782	0.327296	0.015486	4.5177
.80	0.527089	0.493056	0.034033	6.4569
.90	0.751830	0.691790	0.060040	7.9859
1.00	1.000000	0.942143	0.057857	5.7857

We note that the condition (5.4) allows sufficient generality since we can artificially introduce the error resulting from the computation of v^* from (3.1) into f^* via a random error generator.

When no data error was introduced 5 to 6 place accuracy was achieved for $0 \leqslant x \leqslant .7$. In Tables II and III we present sample results of our method of series approximation for various randomly introduced data errors. The variable choices of h_i described in Section 4 were used in all cases. All computations are made for $t = 0.050$ in (5.2).

We noted that a fairly good initial estimate of V for all x from 0 to 1 is obtained using $n = 2$, while for the larger $n = 8$, much better estimates are obtained within the radius of convergence of the series and worse estimates are obtained outside this radius. Using a uniform $h = 0.001$, we obtained better estimates for small x than with variables h_i, but the approximation blew up rapidly for larger x.

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