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

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For the Cauchy problem, \( u_t = u_{xx} \), \( 0 < x < 1 \), \( 0 < t \leq T \), \( u(0, t) = f(t) \), \( 0 < t \leq T \), a direct numerical procedure involving the elementary solution of \( v_t = v_{xx} \), \( 0 < x \), \( 0 < t \leq T \), \( v_x(0, t) = g(t) \), \( 0 < t \leq T \), \( v(0, 0) = 0 \), \( 0 < x \) 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

\[
\begin{align*}
(a) & \quad u_t = u_{xx}, \quad 0 < x < 1, \quad 0 < t \leq T, \\
(b) & \quad u(0, t) = f(t), \quad 0 < t \leq T, \\
(c) & \quad u_x(0, t) = g(t), \quad 0 < t \leq T,
\end{align*}
\]

(1.1)

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

\[
\begin{align*}
(a) & \quad \| f - f^* \| < \epsilon, \\
(b) & \quad \| g - g^* \| < \epsilon,
\end{align*}
\]

(1.2)

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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 $0 < x < 1$, $0 < t \leq T$,

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

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:

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

and a Taylor’s series in $x$ computed from $f - v(0, t)$. Using this approach,
we achieve results in the interval $0 \leq x < 1/\sqrt{2}$, 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

$$u = v + w,$$  \hspace{1cm} (2.1)

where $v$ satisfies

(a) $v_t = v_{xx}$, \hspace{1cm} $0 < x < 1$, \hspace{0.5cm} $0 < t \leq T$,
(b) $v_x(0, t) = g(t)$, \hspace{1cm} $0 < t \leq T$,
(c) $v(x, 0) = 0$, \hspace{1cm} $0 < x$,

and $w$ satisfies

(a) $w_t = w_{xx}$, \hspace{1cm} $0 < x < 1$, \hspace{0.5cm} $0 < t \leq T$,
(b) $w(0, t) = f(t) - v(0, t)$, \hspace{1cm} $0 < t \leq T$,
(c) $w_x(0, t) = 0$, \hspace{1cm} $0 < t \leq T$,
(d) $|w(x, 0)| < M$, \hspace{1cm} $0 < x < 1$.

Since the bounded solution of (2.2) is given by

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

it follows from elementary estimates [1] that

$$|v(x, t)| \leq M_1 \|g\|,$$  \hspace{1cm} (2.5)

where

$$M_1 = \pi^{-1/2}T^{1/2} + 2^{-1}.$$  \hspace{1cm} (2.6)
Now, by constructing an even extension of \( w \), we see that
\[
\begin{align*}
(a) & \quad w_t = w_{xx}, \quad -1 < x < 1, \quad 0 < t \leq T, \\
(b) & \quad w(0, t) = f(t) - v(0, t), \quad 0 < t \leq T, \\
(c) & \quad w_x(0, t) = 0, \quad 0 < t \leq T, \\
(d) & \quad |w(x, 0)| < M, \quad -1 < x < 1, \\
(e) & \quad |w(-1, t)| < M + M_1 \|g\|, \quad 0 < t \leq T, \\
(f) & \quad |w(1, t)| < M + M_1 \|g\|, \quad 0 < t \leq T.
\end{align*}
\]

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
\[
G_\mu = \{ z : -1 < x < 1, \ |y| < \mu(x + 1), \ |y| < \mu(1 - x) \}\]  
for any \( \mu \) satisfying \( 0 < \mu < 1 \). Employing the elementary estimates given in [1, 2], we see that for \( 0 < \delta \leq t \leq T \) and \( z \in G_\mu \),
\[
|w(z, t)| \leq M_2, \quad (2.9)
\]
where
\[
M_2 = M_2(\delta, \mu) = M(\pi \delta)^{-1/2} \exp\{(4\delta)^{-1}\} \left( 1 + \left( \frac{1 + \mu}{1 - \mu} \right)^{1/2} \right) + (M + M_1 \|g\|) \left( \frac{1 + \mu}{1 - \mu} \right)^{1/2}. \quad (2.10)
\]

There is a \( \mu_0 > 0 \) such that the disc \( |z| < \frac{x}{2} \) is contained in \( G_{\mu_0} \). 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,
\[
\frac{1}{n!} \left| \frac{\partial^n w}{\partial x^n} (0, t) \right| \leq M_2 \left( \frac{3}{2} \right)^n, \quad n = 1, 2, 3, \ldots \quad (2.11)
\]
for \( 0 < \delta \leq t \leq T \).

### 3. Numerical Approximation

Let \( v^{**}(x, t) \) denote a numerical approximation of the quadrature
\[
v^{*}(x, t) = \int_0^t g^{*}(\tau) (4\pi(t - \tau))^{-1/2} \exp \left\{ \frac{-x^2}{4(t - \tau)} \right\} d\tau, \quad (3.1)
\]
and let

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

(3.2)

where

\[ w^{**}(0, t) = \{ f(t) - v^{**}(0, t) \} \]  

(3.3)

and \( \Delta_i w^{**}(0, t)/h_i \) 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

\[ u_n^{**}(x, t) = v^{**}(x, t) + w_n^{**}(x, t). \]  

(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

\[ z = v - v^{**}. \]  

(3.5)

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

\[ |z(x, t)| \leq M_1 \varepsilon \]  

(3.6)

for all \( 0 < x < 1 \) and \( 0 < t \leq T \). Clearly, the quadrature approximation can be made as accurately as desired. Hence, there exists a constant \( M_2 \) such that

\[ |v(x, t) - v^{**}(x, t)| \leq M_2 \varepsilon. \]  

(3.7)

Next, we need to estimate the tail of the power series representation for \( w \). Since \( w_2(0, t) = 0 \) implies that every odd \( x \)-derivative of \( w \) vanishes at \( x = 0 \), it follows that for \( n \) odd

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

(3.8)

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

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

(3.9)

where

\[ M_4 = \frac{16}{\pi} M_2. \]  

(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
\[
| w(0, t) - w(0, t) - w***(0, t) | \leq | f(0, t) - v(0, t) - f***(0, t) |
\]
\[
\leq \| f - f^* \| + \sup_{0 < t < T} | v(x, t) - v(x, t) |
\]
\[
\leq \epsilon | M_{3\varepsilon} = M_{3\varepsilon}.
\]

For each \( i = 1, 2, \ldots, (n - 1)/2 \), we see that
\[
\left| \frac{\partial^{2i} w}{\partial x^{2i}} (0, t) - \frac{\Delta_i w(0, t)}{h_i^i} \right|
\]
\[
\leq \left| \frac{\partial^{2i} w}{\partial x^{2i}} (0, t) - \frac{\Delta_i w(0, t)}{h_i^i} \right| + \left| \Delta_i w(0, t) - \Delta_i w**(0, t) \right| \frac{1}{h_i^i},
\]
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 \( i = 1, 2, \ldots, (n - 1)/2 \),
\[
\left| \frac{\partial^{2i} w}{\partial x^{2i}} (0, t) - \frac{\Delta_i w(0, t)}{h_i^i} \right| = \left| \frac{\partial^{2i} w}{\partial t^{2i}} (0, t) - \frac{\Delta_i w(0, t)}{h_i^i} \right|
\]
\[
\leq \sup_{0 < \tau < t} \left| \frac{\partial^{i+1} w}{\partial t^{i+1}} (0, \tau) \right| \frac{1}{2} ih_i
\]
\[
\leq \sup_{0 < \tau < t} \left| \frac{\partial^{i+2} w}{\partial x^{2i+2}} (0, \tau) \right| \frac{1}{2} ih_i
\]
\[
\leq \frac{M_2}{2} (2i + 2)! \left( \frac{3}{2} \right)^{2i+2} ih_i.
\]

Then, using [7, p. 92] and (3.11), we have
\[
\left| \Delta_i w(0, t) - \Delta_i w**(0, t) \right| \frac{1}{h_i^i}
\]
\[
= i! \sum_{s=0}^{i} \frac{w(0, t_s) - w**(0, t_s)}{(t_s - t_0) \cdots (t_s - t_{s-1}) (t_s - t_{s+1}) \cdots (t_s - t_i)}
\]
\[
\leq i! \frac{1}{h_i^i} \sum_{s=1}^{i} | w(0, t_s) - w**(0, t_s) |
\]
\[
\leq \frac{M_3(i + 1)! \epsilon}{h_i^i}.
\]
Combining (3.12)–(3.14) we see that for each \(i = 1, 2, \ldots, (n - 1)/2\),

\[
\left| \frac{\partial^2 w}{\partial x^{2i}} (0, t) - \frac{\Delta w^{**}(0, t)}{h_i^i} \right| \leq \frac{M_5}{2i} (2i + 2)! \left( \frac{3}{2} \right)^{2i+2} i h_i + \frac{M_5 (i + 1)! \varepsilon}{h_i^i}.
\]

(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 \(h_i\),

\[
h_i^* = \left[ \frac{2M_5(i + 1)! \varepsilon}{M_5(2i + 2)! \left( \frac{3}{2} \right)^{2i+2}} \right]^{1/(i+1)}.
\]

(3.16)

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

\[
\left| \frac{\partial^2 w}{\partial x^{2i}} (0, t) - \frac{\Delta w^{**}(0, t)}{h_i^i} \right| \leq M_5(2i + 2)! \left( \frac{3}{2} \right)^{2i+2} i \left[ \frac{2M_5(i + 1)! \varepsilon}{M_5(2i + 2)! \left( \frac{3}{2} \right)^{2i+2}} \right]^{1/(i+1)}
\]

(3.17)

\[
\leq i M_5(2i + 2)! \left( \frac{3}{2} \right)^{2i+2} [M_5 \varepsilon]^{1/(i+1)},
\]

where

\[
M_6 = 2M_5/M_2.
\]

(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 \(0 \leq x \leq \frac{1}{2}, \delta \leq t \leq T\),

\[
|w_n(x, t) - u^{**}(x, t)| \leq |w(0, t) - u^{**}(0, t)| + \sum_{i=1}^{(n-1)/2} \left| \frac{\partial^2 w}{\partial x^{2i}} (0, t) - \frac{\Delta w^{**}(0, t)}{h_i^i} \right| \left( \frac{x^{2i}}{(2i)!} \right)
\]

\[
\leq M_5 \varepsilon + (n + 1)^2 \sum_{i=1}^{(n-1)/2} M_7 \left( \frac{3}{2} x^2 \right)^i \varepsilon^{1/(i+1)}
\]

\[
\leq M_5 \varepsilon + M_6(n + 1)^3 \varepsilon^{1/(n+1)}.
\]

(3.19)

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

\[
|u(x, t) - u^{**}(x, t)| = |v(x, t) + w(x, t) - v^{**}(x, t) - w_n^{**}(x, t)|
\]

\[
\leq |v(x, t) - v^{**}(x, t)| + |w_n(x, t) - w_n^{**}(x, t)|
\]

\[
+ \left| \sum_{i=-(n+1)/2}^{\infty} \frac{\partial^2 w}{\partial x^{2i}} (0, t) \left( \frac{x^{2i}}{(2i)!} \right) \right|
\]

\[
\leq M_{10} (n + 1)^3 \varepsilon^{1/(n+1)} + M_6 \left( \frac{3}{2} x \right)^n + 1
\]

(3.20)
for all $0 \leq x \leq \frac{1}{2}$, $\delta \leq t \leq T$. We see that if we choose

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

in (3.20), then

$$u(x, t) - u^*(x, t) \leq M_0 \left( \frac{\log \epsilon^{-1}}{\log(\frac{3}{2}x)^{-1}} \right)^{3/2} \exp \left[ - \left( \log \epsilon^{-1} \log \left( \frac{3}{2}x \right)^{-1} \right)^{1/2} \right] + M_4 \exp \left[ -(\log \epsilon^{-1} \log(\frac{3}{2}x)^{-1})^{1/2} \right].$$

Using the simple estimate that

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

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

$$n = \left\lceil \frac{\log \epsilon^{-1}}{\log(\frac{3}{2}x)^{-1}} \right\rceil^* 1,$$

where $\lceil x \rceil$ 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 $2M_5/M_2$.

<table>
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<tr>
<th>$i$</th>
<th>0.1</th>
<th>0.01</th>
<th>0.001</th>
<th>0.0001</th>
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<tr>
<td>1</td>
<td>0.0406</td>
<td>0.0128</td>
<td>0.0041</td>
<td>0.0013</td>
</tr>
<tr>
<td>2</td>
<td>0.0418</td>
<td>0.0194</td>
<td>0.0090</td>
<td>0.0042</td>
</tr>
<tr>
<td>3</td>
<td>0.0390</td>
<td>0.0220</td>
<td>0.0123</td>
<td>0.0070</td>
</tr>
<tr>
<td>4</td>
<td>0.0356</td>
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<td>0.0142</td>
<td>0.0090</td>
</tr>
<tr>
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<td>0.0324</td>
<td>0.0221</td>
<td>0.0150</td>
<td>0.0103</td>
</tr>
<tr>
<td>6</td>
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<td>0.0153</td>
<td>0.0110</td>
</tr>
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<td>0.0203</td>
<td>0.0153</td>
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<td>0.0146</td>
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</tr>
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<td>10</td>
<td>0.0216</td>
<td>0.0175</td>
<td>0.0142</td>
<td>0.0115</td>
</tr>
</tbody>
</table>

We conclude that three different choices of $h_i$ will suffice for each choice of $2M_5/M_2$ if we consider $n \leq 10$ (20 terms in our power series). In particular for $2M_5/M_2 = 0.0001$, 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

\[(a)\quad V_t = V_{xx}, \quad 0 < x < 1, \quad 0 < t,\]
\[(b)\quad V(1, t) = 1, \quad 0 < t,\]
\[(c)\quad V(x, 0) = 0, \quad 0 < x < 1.\]  

We see that the function

\[ V(x, t) = 1 + 2 \sum_{n=0}^{\infty} \exp\left(-\frac{(2n+1)^2 \pi^2 t}{4}\right) F(n, x) \]
where
\[ F(n, x) = \left[ \frac{(-1)^{n+1} 2}{(2n + 1) \pi} \right] \cos \left( \frac{(2n + 1) \pi x}{2} \right) \]  
(5.3)
is a solution to the boundary value problem defined by (5.1) satisfying, in addition, the condition
\[ V_x(0, t) = 0. \]  
(5.4)

| TABLE II |
|-----------------|-----------------|-----------------|
|                | 0.1% Data Error | Truncation n = 2 |
| X              | V(x, t)         | u**(x, t)       | [V(x, t)−u**(x, t)] | % Error  |
| 0.10           | 0.004931        | 0.004923        | 0.000008           | 0.1592   |
| 0.20           | 0.011560        | 0.011478        | 0.000082           | 0.7087   |
| 0.30           | 0.026896        | 0.026332        | 0.000564           | 2.0976   |
| 0.40           | 0.057789        | 0.055378        | 0.002411           | 4.1726   |
| 0.50           | 0.113848        | 0.106866        | 0.006982           | 6.1325   |
| 0.60           | 0.205904        | 0.191406        | 0.014498           | 7.0413   |
| 0.70           | 0.342782        | 0.321961        | 0.020821           | 6.0741   |
| 0.80           | 0.527089        | 0.513855        | 0.013234           | 2.5108   |
| 0.90           | 0.751830        | 0.784767        | 0.032937           | 4.3810   |
| 1.00           | 1.000000        | 1.154736        | 0.154736           | 15.4736  |

| TABLE III |
|-----------------|-----------------|-----------------|
|                | 0.1% Data Error | Truncation n = 8 |
| X              | V(x, t)         | u**(x, t)       | [V(x, t)−u**(x, t)] | % Error  |
| 0.10           | 0.004931        | 0.004924        | 0.000007           | 0.1475   |
| 0.20           | 0.011560        | 0.011513        | 0.000047           | 0.4074   |
| 0.30           | 0.026896        | 0.026686        | 0.000210           | 0.7806   |
| 0.40           | 0.057789        | 0.057031        | 0.000758           | 1.3110   |
| 0.50           | 0.113848        | 0.111541        | 0.002307           | 2.0266   |
| 0.60           | 0.205904        | 0.199647        | 0.006257           | 3.0387   |
| 0.70           | 0.342782        | 0.327296        | 0.015486           | 4.5177   |
| 0.80           | 0.527089        | 0.493056        | 0.034033           | 6.4569   |
| 0.90           | 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 $0 < x < .7$. 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 $x$.

REFERENCES

11. JIM DOUGLAS, Jr., private communication to the Authors.