FINITE DIFFERENCE METHODS FOR APPLROXIMATING SOLUTIONS TO THE HEAT EQUATION

THESIS

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By

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This paper is concerned with finite difference methods for approximating solutions to the partial differential heat equation.

The first chapter gives some introductory background into the physical problem, then motivates three finite difference methods. Chapters II through IV provide statements and proofs for the theorems used in the methods of Chapter I. The final Chapter, V, provides conclusions and an indication of future work. An appendix includes the computer codes written by the author with numerical results.
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CHAPTER I

MOTIVATION OF METHODS

Introduction

This paper is concerned for the most part with some finite difference methods for approximating solutions to the pure heat equation. It is hoped that some insight will be gained into ways one might continue this quest or, for that matter, approach new problems.

The first chapter discusses the partial differential heat equation and motivates three finite difference methods for approximating its solution. Chapters II through IV provide definitions, statements of theorems used in the methods of Chapter I, proofs and references. The final Chapter V, provides conclusions and an indication of future work. In the Appendix are computer codes for the numerical methods described in Chapter I and some numerical results which include comparisons with known solutions. The ideas and theorems in this paper are derived from the literature and from courses, both graduate and undergraduate, taken by the author.

For the most part the theorems that are stated are kept fairly specialized to their use. However, not many changes should be required for more general statements and proofs.
The Physical Problem

The mathematical formulation of a scientific problem often involves rates of change with respect to two or more variables. If we consider an insulated bar of length, say L, the theory of heat conduction inspires a mathematical expression for the problem of predicting the temperature distribution along the bar at a certain time. Suppose the temperatures at the ends of the bar (where there is no insulation) are known for some extended period of time, perhaps kept constant, and the temperatures along the bar are known at some instant, which may be considered as time zero.

The temperature distribution along the bar at time zero provides a set of initial conditions, and temperatures at the ends of the bar over a specified time period provide boundary conditions for the partial differential equation

\[ u_1 = u_{22} \]

where \( u(t,x) \) is the temperature of the bar at time \( t \) and position \( x \), \( 0 \leq x \leq L \), \( u_1 \) is the first derivative with respect to the time variable and \( u_{22} \) is the second derivative with respect to the space variable.

Although it is possible to arrange boundary and initial conditions so that a closed form solution is available, since the physical world does not limit itself to closed form solutions it is most likely that, even assuming precise boundary and initial conditions for \( u_1 = u_{22} \), the solutions are
unknown or at least not expressible in any current closed form notation.

To pose a specific problem consider the length of the bar to be a unit length of \( L = 1 \), the boundary conditions to be zero (that is the ends of the bar are kept at zero degrees centigrade) and the initial condition (heat distribution at time zero) to be given by the single variable function \( h \) where \( h(x) = u(0,x) = \sin \pi x, \, 0 < x < 1 \). This would describe a situation where heat is applied to the middle of the bar, resulting in a temperature distribution symmetrical about the center point.

The heat source is removed from the insulated bar at time zero. The temperature along the bar is sought after some appropriate interval of time.

In this example the initial and boundary conditions provide a closed form solution which invites comparison between numerical estimates and the actual solution given uniquely by:

\[
u(t,x) = e^{-\pi^2 t} \sin \pi x
\]

Here \( u(0,x) = \sin \pi x, \, u(t,0) = 0 = u(t,1) \) for \( t \geq 0 \), and \( u_1(t,x) = -\pi^2 e^{-\pi^2 t} \sin \pi x = u_{22}(t,x) \).

The problem of estimating \( u(t,x) \) for any \( x \in [0,1] \) and a specified positive number \( t \) can be changed into a finite problem. The space interval \([0,1]\) representing the bar of unit length 1 is subdivided into \( m \) pieces of equal length. The resulting partition forms a vector in \( \mathbb{R}^{m+1} \):
\( X = (x_1, x_2, \ldots, x_{m+1}) \). If we let \( Dx = 1/m \) then

\[ x_{k+1} = x_k + Dx, \quad k = 1, 2, \ldots, m. \]

The finite time interval \([0, t]\) is subdivided into \( n \) pieces of equal length. We let \( \delta = t/n \) and note

\[ t_{i+1} = t_i + \delta, \quad i = 1, 2, \ldots, n. \]

The domain of \( u \), which is \([0, \infty) \times [0, 1]\) is first restricted to the rectangle (plus interior) \( R = [0, t] \times [0, 1] \). Then the finite grid produced by the time and space partitions is considered.

The range of \( u \) restricted to a domain grid is a collection of vectors, each representing the temperatures along the space partition.

We let \( \overline{Y}_1 = (y_1(1), y_1(2), \ldots, y_1(m+1)) = (u(0,0), u(0,x_2), \ldots, u(0,1)) \) denote the initial vector for which the coordinates are known and \( \overline{Y}_i = (y_i(1), y_i(2), \ldots, y_i(m+1)) \quad i = 2, 3, \ldots, n+1, \)
where \( y_i(k) \) is the estimated value of \( u(t_i, x_k) \). If \( h(x) = \sin \pi x = u(0,x) \) for \( x \in [0,1] \), then \( y_1(k) = \sin ((k-1)Dx \pi), \quad k = 1, 2, \ldots, m. \)

Since \( y_i(1) = y_i(m+1) = 0 \) for each \( i \), it follows that the needed vector to estimate is \( \overline{Y}_i = (y_i(2), y_i(3), \ldots, y_i(m)), \)
which is \( \overline{Y}_i \) minus the first and last coordinates representing the zero degree boundary values.

The initial condition vector \( \overline{Y}_1 \) is used to obtain an estimate for \( \overline{Y}_2 \) at the first intermediary time step \( t/n = \delta \) and those entries are then used to proceed to an approximation
for $Y_2$, and so on. When $Y_{n+1}$ is computed in terms of $Y_n$, the estimated values at time $t$ are reached.

Closeness to the actual solution can be expected to vary with the method; but the general idea is that the numerical approximations are good when $Dx$ and $\delta$ are "appropriately small."

A comment about the notation: a vector in $\mathbb{R}^{m+1}$ is denoted by $\bar{Y}=y_1, y_2, \ldots, y_{m+1}$ rather than by $y_0, y_1, \ldots, y_m$. The vector $Y$ in $\mathbb{R}^m$ consisting of $\bar{Y}$ minus the first and last coordinates is then expressed as $Y=y_2, y_3, \ldots, y_m$, which may look a bit peculiar. This merely facilitates "relating to" the FORTRAN program codes which do not allow for 0 subscript. As it turns out, in this paper the first coordinate of a full vector in $\mathbb{R}^{m+1}$ happens to be zero but the programs should generalize with relatively few changes. For example one might consider non-zero boundary conditions.

Method I

Looking to the partial differential equation $u_1 = u_{22}$ for inspiration, and assuming $\delta$ and $Dx$ are "small", we let $(y_2(2) - y_1(2))/\delta$ approximate $u_1(t_2, x_2)$. Then $y_2(2) - y_1(2) + \delta u_1(t_2, x_2) = y_1(2) + \delta u_{22}(t_2, x_2)$. 
An explicit expression for estimating $u_{22}(t_2, x_2)$ can be obtained in terms of the initial vector $Y_1$:

Let $\frac{(y_1(2) - y_1(1))}{Dx} \approx u_2(0, x_{1.5})$ and $\frac{(y_1(3) - y_1(2))}{Dx} \approx u_2(0, x_{2.5})$. Then $(1/Dx)(y_1(3) - y_1(2))/Dx - (y_1(2) - y_1(1))/Dx)$, which simplifies to $(y_1(3) - 2y_1(2) + y_1(1))/(Dx)^2$, approximates $u_{22}(0, x_2)$, which in turn approximates $u_{22}(t_2, x_2)$.

For purposes of illustration let us divide the space interval into $m = 5$ equal subintervals. In matrix vector form

$$\bar{A} Y_1 = \frac{1}{Dx}$$

$$= \frac{1}{Dx} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} y_1(1) \\ y_1(2) \\ y_1(3) \\ y_1(4) \\ y_1(5) \\ y_1(6) \end{pmatrix} = 1/Dx \begin{pmatrix} y_1(2) - y_1(1) \\ y_1(3) - y_1(2) \\ y_1(4) - y_1(3) \\ y_1(5) - y_1(4) \\ y_1(6) - y_1(5) \end{pmatrix}$$

where $A$ is the linear transformation represented by the $5 \times 4$ $[m \times (m-1)]$ matrix that takes first differences along $Y_1$. 
Now we let
\[ QY_1 = BA Y_1 = (1/Dx) \begin{pmatrix} -1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 1 \\ \end{pmatrix} (1/Dx) \begin{pmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ \end{pmatrix} \begin{pmatrix} y_1(2) \\ y_1(3) \\ y_1(4) \\ y_1(5) \\ \end{pmatrix} \]
\[ = (1/Dx)^2 \begin{pmatrix} -2 & 1 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 0 & 0 & 1 & -2 \\ \end{pmatrix} \begin{pmatrix} y_1(2) \\ y_1(3) \\ y_1(4) \\ y_1(5) \\ \end{pmatrix} \]
\[ = (1/Dx)^2 \begin{pmatrix} y_1(3) - 2y_1(2) + y_1(1) \\ y_1(4) - 2y_1(3) + y_1(2) \\ y_1(5) - 2y_1(4) + y_1(3) \\ y_1(6) - 2y_1(5) + y_1(4) \\ \end{pmatrix} \sim \begin{pmatrix} u_{22}(0,x_2) \\ u_{22}(0,x_3) \\ u_{22}(0,x_4) \\ u_{22}(0,x_5) \\ \end{pmatrix} \]

where \( Q = BA \) takes second differences along \( Y_1 \).

Thus, we have \( Y_2 = Y_1 + \delta Q Y_1 = (I + \delta Q)Y_1 \). Similarly,
\[ Y_3 = (I + \delta Q)Y_2 = (I + \delta Q)(I + \delta Q)Y_1 = (I + \delta Q)^2 Y_1 , \]
and
\[ Y_{n+1} = (I + \delta Q)Y_{n-1} = \ldots = (I + \delta Q)^n Y_1 . \]

If our space were \( \mathbb{R} \), the real numbers, the preceding expression would indicate a method for solving a single first order ordinary differential equation. Instead, we are in \( \mathbb{R}^{m-1} \) and the partial differential equation \( u_1 = u_{22} \) over \( [0,t] \times [0,1] \) (with zero boundary conditions and a designated initial condition function \( h \)) can be approximated by a system of ordinary differential equations. Selecting a positive integer \( m \) and defining \( Dx = 1/m \), let us refer to Theorem 1 of Chapter II for the existence of a unique sequence of real valued functions \( g_1, g_2, \ldots, g_{m+1} \) with domain \([0,t]\).
where

1) each of \( g_1 \) and \( g_{m+1} \) is the constant zero function,

2) \( g'_k = (g_{k+1} - 2g_k + g_{k-1})/(Dx)^2 \) \( k = 2, 3, \ldots, m \) and

3) \( g_k(0) = h(x_k) \) where \( k = 1, 2, \ldots, m + 1 \) and \( x_k = (k-1)Dx \).

With reference to Theorem 1 we let \( f(r) \) denote 
\((g_2(r), g_3(r), \ldots, g_m(r)), r \in [0, t]\). Then \( f'(r) = Qf(r) \) where \( Q \) is the linear transformation associated with the constant 
\((m - 1) \times (m - 1)\) matrix that transforms \( f \) to \( f' \).

Since \( \int_0^t f' = f(t) - f(0) \) we note that 
\[ f(t) = f(0) + Q \int_0^t f. \]

Let \( Y_1 = (h(x_2), h(x_3), \ldots, h(x_m)) \) and observe that \( Y_1 = f(0) \).

Theorems 2 through 4 of Chapter II demonstrate that \((I + \delta Q)^n Y_1\) converges to \( f(t) \) as \( n \to \infty \):
\[ \lim_{n \to \infty} (I + \frac{t}{n} Q)^n Y_1 = f(t) = f(0) + Q \int_0^t f. \]

Although the explicit method is a simple one and therefore desirable to have on hand (especially in a non-linear situation) it has an unfortunate disadvantage in that if \( Dx \) is chosen small for the sake of accuracy the time interval must be divided into a very large number of pieces which then require a great number of calculations. In fact, the process is only valid when the ratio \( \delta/(Dx)^2 \) is in \((0, 1/2]\). See Chapter 1 of reference (4), Chapters 1 and 3 of reference (6).
Method II

Referring to the way the preceding explicit method was constructed we can derive a more stable implicit method that does not suffer this disadvantage.

Again, let \((y_2(k) - y_1(k))/\delta - u_1(t_2, x_k), k = 2, 3, \ldots, m\).

In the explicit case \(u_2(t_2, x_k)\) was approximated with an approximation for \(u_{22}(t_1, x_k)\) - namely \((y_1(k+1) - 2y_1(k) + y_1(k-1))/(Dx)^2\) - thus taking immediate advantage of the assumed initial data.

For an implicit method we shall use \((y_2(k+1) - 2y_2(k) + y_2(k-1))/(Dx)^2\) to estimate \(u_{22}(t_2, x_k)\); that is \(Y_2\) is no longer expressed entirely in terms of \(Y_1\). Instead,

\[ y_2(k) = y_1(k) + \delta(y_2(k+1) - 2y_2(k) + y_2(k-1))/(Dx)^2 \]

which amounts to

\[ Y_2 = Y_1 + \delta Q Y_2 \]

where \(Q = BA\); therefore \(Y_2 - \delta Q Y_2 = Y_1\), \((I - \delta Q)Y_2 = Y_1\), and so we finally have an expression for \(Y_2\) in terms of \(Y_1\):

\[ Y_2 = (I - \delta Q)^{-1}Y_1. \]

Now we note that \((I - \delta Q) = (I + \delta(-BA))\). Again, using the example of \(m = 5\), \(-Q = -BA\) is associated with the following product of matrices:
Observing that $-B = A^*$ is the transpose of $A$ and that $\delta > 0$, it is shown (lemma 7, Chapter III) that $(I - \delta Q) = (I + \delta A^* A)$ is, in fact, invertible.

We now use $Y_2 = (I - \delta Q)^{-1}Y_1$ to estimate $(u(t_2, x_2), u(t_2, x_3), \ldots, u(t_2, x_m))$. The vector $Y_3$ is then calculated in terms of $Y_2$:

$$Y_3 = (I - \delta Q)^{-1}Y_2 = (I - (t/n)Q)^{-2}Y_1,$$

and so to $Y_{n+1} = (I - (t/n)Q)^{-n}Y_1$.

Let us consider the first of the iterative steps.

Finding the vector $Y_2$, where $Y_1$ is known and $(I - \delta Q)Y_2 = Y_1$, amounts to solving a system of $m - 1$ (4 in our example) simultaneous equations.

Let $\alpha = \delta/(Dx)^2$ and $\beta = (1 + 2\alpha)$. Then $(I - \delta Q)Y_2 = (I + \delta(-Q))Y_2 = Y_1$ is expressed in matrix-vector form as:
\[
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix} + \alpha \begin{pmatrix}
2 & -1 & 0 & 0 \\
-1 & 2 & -1 & 0 \\
0 & -1 & 2 & -1 \\
0 & 0 & -1 & 2
\end{pmatrix} (Y_2) =
\]

\[
\begin{pmatrix}
\beta - \alpha & 0 & 0 \\
-\alpha & \beta - \alpha & 0 \\
0 & -\alpha & \beta \\
0 & 0 & -\alpha & \beta
\end{pmatrix} \begin{pmatrix}
y_2(2) \\
y_2(3) \\
y_2(4) \\
y_2(5)
\end{pmatrix} = \begin{pmatrix}
y_1(2) \\
y_1(3) \\
y_1(4) \\
y_1(5)
\end{pmatrix}
\]

which conveniently leaves us with a tridiagonal matrix to invert. See Chapter 2 of (2).

Method III

In the explicit case described previously \((Y_2 - Y_1)/\delta = QY_1\) provided us with \(Y_2 = Y_1 + \delta QY_1 = (I + \delta Q)Y_1\).

In the implicit case \((Y_2 - Y_1)/\delta = QY_2\) resulted in \(Y_1 = (I - \delta Q)Y_2\) and hence \(Y_2 = (I - \delta Q)^{-1}Y_1\).

Crank and Nicolson (1947) used an implicit method superior to the one just described (reference [6], p. 17). In the CN (Crank-Nicolson) case the average of \(Y_1\) and \(Y_2\) is used. This amounts to allowing \((Y_2 - Y_1)/\delta\) to approximate the slope of \(u\) at \((t_1 + t_2)/2\). The appealing idea lives up to expectation and provides better estimates than the "end point" methods:

\((Y_2 - Y_1)/\delta = Q(Y_1 + Y_2)/2, Y_2 - Y_1 = (\delta/2)QY_1 + (\delta/2)QY_2,\)

\((I - (\delta/2)Q)Y_2 = (I + (\delta/2)Q)Y_1, Y_2 = (I - (\delta/2)Q)^{-1}(I + (\delta/2)Q)Y_1,\)

\(Y_3 = (I - (\delta/2)Q)^{-1}(I + (\delta/2)Q)Y_2 = (I - (\delta/2)Q)^{-1}(I + (\delta/2)Q)(I - (\delta/2)Q)^{-1}(I + (\delta/2)Q)Y_1 = (I - (\delta/2)Q)^{-2}(I + (\delta/2)Q)^2\) [since \((I + (\delta/2)Q)\)
commutes with \((I - (\delta/2)Q)\) it follows that \((I + (\delta/2)Q)\) commutes with \((I - (\delta/2)Q)^{-1}\), and

\[
Y_{n+1} = (I - (\delta/2)Q)^{-n} (I + (\delta/2)Q)^n Y_1
\]

\[
= ((I - (t/2n)Q)^{-1})^n (I + (t/2n)Q)^n Y_1.
\]

Again, as with the simpler implicit case, we are left with what amounts to a tridiagonal matrix: \((I - (\delta/2)Q)\).
CHAPTER BIBLIOGRAPHY


CHAPTER II

AN EXPPLICIT METHOD

As indicated in the introduction the main item of business in this chapter is to show the explicit method really works; that is to say (we refer to previous notation):

1) \((I + \delta Q)^n Y_1\) converges as \(n \to \infty\),

2) \(\lim_{n \to \infty} (I + \delta Q)^n Y_1\) fits the underlying differential equation, and

3) the difference between the limit and the actual solution (at the chosen finite number of grid points) is satisfactorily close. In other words, we would like a "workable bound on an error estimate."

Before proceeding with all of this it is appropriate to show the existence of a solution to the approximating problem \(u_1 = u_{22}\) over a selected rectangular grid given an initial value vector and zero boundary conditions.

Throughout this paper we shall let \(m\) be a positive integer \(\geq 2\), \(Dx = 1/m\), and \(x_k = (k - 1)Dx\) \(k = 1, 2, \ldots, m + 1\).

Some of the lemmas follow the theorems.

Definition 1: Let \(t > 0\), \(g_k\) denote a continuous real valued function on \([0, t]\), \(k = 1, 2, \ldots, m + 1\), and

\(f = (g_1, g_2, \ldots, g_{m+1})\). Then \(f' = (g'_1, g'_2, \ldots, g'_{m+1})\) and

\(\int_0^T f = (\int_0^T g_1, \int_0^T g_2, \ldots, \int_0^T g_{m+1})\) \(r \in [0, t]\).
Definition 2: Let $Q$ denote the member of $L(R^{m-1}, R^{m-1})$ such that if $Y \in R^{m-1}$, $Y = (y_2, y_3, \ldots, y_m)$ then $QY = Z$ where

$z_2 = 1(Dx)^2(-2y_2 + y_3),$

$z_k = 1/(Dx)^2(y_{k-1} - 2y_k + y_{k+1})$ for $k = 3, 4, \ldots, m - 1$, and

$z_m = 1/(Dx)^2(y_{m-1} - 2y_m).$

Theorem 1 (existence): Let $t > 0$ and $h$ denote a continuous real valued function on $[0,1]$ such that $h(0) = 0 = h(1)$.

There exists a unique sequence $T = g_1, g_2, \ldots, g_{m+1}$ of real valued functions on $[0,t]$ such that $g_1 = 0 = g_{m+1}$, $g_k(0) = h(x_k)$ and

$g_k' = (1/Dx)^2(g_{k-1} - 2g_k + g_{k+1})$ if $k = 2, 3, \ldots, m$.

Proof: Let $w = |Q|$. For all $r \in [0,t]$ let

$f_0(r) = (h(x_2), h(x_3), \ldots, h(x_m))$ and given $n = 0, 1, 2, \ldots$, $r \in [0,t]$ let $f_{n+1}(r) = f_0(0) + \int_0^r Qf_n$.

Consider the sequence of functions $F_0, F_1, F_2, \ldots$ on $[0,t]$ into $R^{m-1}$ defined by $F_n = f_{n+1} - f_n$, $n$ a non-negative integer.

Then

$F_n(r) = f_{n+1}(r) - f_n(r) = f_0(0) + \int_0^r Qf_n - f_0(0) - \int_0^r Qf_{n-1}$

$= Q \int_0^r f_n - f_{n-1} = Q \int_0^r F_{n-1}$ for $n = 1, 2, \ldots$.

Let $L = ||F_0||_{[0,t]}$. Observe that $||F_1|| = ||Qf_0|| \leq ||Q|| \int_0^r F_0 \leq ||Q|| \int_0^r ||F_0||$ (since $\sum_{k=1}^n (t_{k+1} - t_k) F_0(s_k) \leq \sum_{k=1}^n (t_{k+1} - t_k) ||F_0(s_k)||$ where $\{s_k\}_{k=1}^n$ is an interpolating sequence for the $t_{n+1}$ partition). Hence

$||F_1|| \leq ||Q|| \int_0^r ||F_0|| = w \int_0^r L = L wr$ and

$||F_2|| \leq ||Q|| \int_0^r ||F_1(s)|| ds \leq w \int_0^r (L w s) ds = w L w \int_0^r s ds = L w^2 r^2/2 = L(w r)^2/2.$
By induction $\|F_n(r)\| \leq L(\omega r)^n/n!$, $r \in [0,t]$.

It follows that for integers $n \geq N > 0$

$$\|f_n(r) - f_n(r)\| \leq \sum_{k=N}^{n-1} \|f_k+1(r) - f_k(r)\| = \sum_{k=N}^{n-1} \|F_k(r)\|$$

$$\leq \sum_{k=N}^{n-1} L(\omega r)^k/k! = \sum_{k=1}^{M/2^k} \text{(for some } M > 0, \text{ using lemma 1, to follow)} \leq \sum_{F=1}^{\infty} M/2^k = M.$$

Let $\varepsilon > 0$ and $N_\varepsilon$ be a positive integer so that

$$\sum_{k=N_\varepsilon}^{\infty} (\omega t)^k/k! < \varepsilon/L \text{ all } n \geq N \geq N_\varepsilon.$$ Then if $n \geq N \geq N_\varepsilon$ and

$$r \in [0,t] \|f_n(r) - f_N(r)\| < L \sum_{k=N}^{n-1} \omega r^k/k! \leq L \sum_{k=1}^{M/2^k} \text{(for some } M > 0, \text{ using lemma 1, to follow)} \leq \sum_{F=1}^{\infty} M/2^k = M.$$

Observing that $f_1, f_2, \ldots$ is a uniform Cauchy sequence and hence converges uniformly on $[0,t]$ (3, p. 277), we let $f$ denote the uniform and hence the pointwise, limit of $f_1, f_2, \ldots$ on $[0,t]$. Note that $f$ is continuous (5, p. 47).

Hence

$$f(r) = \lim_{n \to \infty} f_n(r) = \lim_{n \to \infty} \left(f_0(0) + \int_0^r Q f_{n-1}\right)$$

$$= \lim_{n \to \infty} \left(f_0(0) + Q \int_0^r f_{n-1}\right) = f_0(0) + \lim_{n \to \infty} Q \int_0^r f_{n-1}$$

$$= f_0(0) + Q f$$

(since $f_1, f_2, \ldots$ converges uniformly to $f$ on $[0,t]$; (5, p. 280), and $f'(r) = Q f(r)$.

Let $g_1 = 0 = g_{m+1}$ over $[0,t]$ and $(g_2(r), g_3(r), \ldots, g_m(r))$ denote $f(r)$. Then $f'(r) = (g_2(r), g_3(r), \ldots, g_m(r)) = Q(g_2(r), g_3(r), \ldots, g_m(r)) = Q f(r)$. Observe that

$$g_k'(r) = (1/Dx)^2 (g_{k-1}(r) - 2g_k(r) + g_{k+1}(r)) \quad k = 2,3,\ldots,m$$ and
\[ f(0) = (g_2(0), g_3(0), \ldots, g_m(0)) = f_0(0) + Q \int_0^0 f = f_0(0) = (h(x_2), h(x_3), \ldots, h(x_m)). \]

Uniqueness: We suppose \( f^* = g_1^*, g_2^*, \ldots, g_{m+1}^* \) is a sequence of continuous real valued functions on \([0, t]\) and \( f^* = (g_2^*, g_3^*, \ldots, g_m^*) \) so that \( f^*(0) = f(0) \) and \( f^*(r) = f^*(0) + Q \int_0^r f^*, \, r \in [0, t] \). Then \((f^*-f)(r) = f(0) + Q \int_0^r (f^*-f) = Q \int_0^r (f^*-f), \quad \|f^*-f)(r)\| = \|Q|\int_0^r (f^*-f)| \leq |Q| \int_0^r (f^*-f)| \leq |Q| \int_0^r (f^*-f)(s) | ds. \]

Let \( H(r) = \|f^*-f)(r)\| \). Then \( |H(r)| \leq |Q| \int_0^r |H| | ds \) and it follows from lemma 3 that \((f^*-f)(r) = 0 \) each \( r \); hence \( f^* = f \).

Lemma 1: Given \( t > 0, L > 0, \omega > 0 \) there exists \( M > 0 \) so that \( L(\omega r)^n/n! < M/2^n, \, n \in \mathbb{Z}^+, \, r \in [0, t] \).

Proof. Let \( m \) denote the smallest integer so that 1) \( m > 2\omega t, \) 2) \( m > (2\omega t)^2 \) and 3) \( m > L(2\omega t) \).

Then since \( L(2\omega t)^n/n! \to 0 \) as \( n \to \infty \) it follows that \( L(2\omega r)^n/n! \leq L(2\omega t)^n/n! < 1 \) for \( n \geq 2m-1 \). Let \( M \geq 1 \) and \( M > \max\{L(2\omega t)^n/n! : n = 1, 2, \ldots, 2m-1\} \). Then \( L(2\omega r)^n/n! < M \) \( n \leq 2m-2 \) and \( L(2\omega r)^n/n! < 1 \leq M, \, n \geq 2m-1 \).

Lemma 2: If \( f_0, f_1, \ldots \) is a sequence of real valued functions on \([0, t], \, \omega > 0, \, |f_n(r)| \leq \omega |f_0| f_{n-1}|, \) and \( L = \text{u.b. of } |f_0| \) over \([0, t], \) then \( |f_n(r)| \leq L(\omega r)^n/n! \), \( r \in [0, t], \, n = 1, 2, \ldots \).

Proof. \( |f_1(r)| = \omega |f_0| \int_0^r f_0| = wL r, \, |f_2(r)| = w \int_0^r |f_1| = wL \int_0^r (\omega L s) ds = L\omega^2 r^2/2 = L(\omega r)^2/2! \), etc.
Lemma 3. If \( f \) is a continuous real valued function on \([0,t]\) such that \( |f(r)| \leq w \int_0^r |f| \) each \( r \in [0,t] \) then \( f = 0 \).

Proof. This is a corollary to lemma 2 allowing \( f = f_n \) each \( n \) then \( |f(r)| \leq L(wt)^n/n! \) each \( n \); hence \( f(r) = 0 \).

Definition 3. Denote by \( M \) the function from \([0,t]\) into the set of transformations from \( \mathbb{R}^{m-1} \) into \( \mathbb{R}^{m-1} \) so that if \( Y \in \mathbb{R}^{m-1} \) and \( r \in [0,t] \) then \( M(r)Y = Z_y(r) \) where \( Z_y = (z_2, z_3, \ldots, z_m) \) is the unique ordered collection of functions on \([0,t]\) such that \( Z'_y = QZ \) and \( Z_y(0) = Y \). Note that \( M(0) = I \), \( M(r)Y_1 = f(r) \) (as in Theorem 1), and \( M(t)Y_1 = f(t) = Y_{n+1} \).

Following from the above definition of \( M \) and from the uniqueness of Theorem 1 are the following facts which are used throughout much of the rest of this paper.

Fact 1: \( M(r) \) is linear.

Proof. Suppose \( X, Y \in \mathbb{R}^{m-1} \), \( a \in \mathbb{R} \). \( M(r)(X + Y) = a \)
\( Z_{x+y}(r) \) where \( a Z_{x+y}(0) = a (X + Y) \) and \( a Z'_y = a QZ_{x+y} = \)
\( Q (a Z_{x+y}) \).
\( M(r)(aX) + M(r)(aY) = h(r) = Z_{ax}(r) + Z_{ay}(r) \) where
\( h(0) = Z_{ax}(0) + Z_{ay}(0) = (aX + aY) = a(X + Y) \) and \( h' = Z'_{ax} + Z'_{ay} = \)
\( Q Z_{ax} + Q Z_{ay} = Q(Z_{ax} + Z_{ay}) = Qh \). By uniqueness \( a M(r)(X+Y) = \)
\( h(r) = M(r)(aX) + M(r)(aY) \).

Fact 2: \( M(r)M(s) = M(r+s) \), \( r, s \) in \([0,t]\).

Proof. Let \( X \in \mathbb{R}^{m-1} \) and \( s \) denote a fixed number in \([0,t]\). Then \( M(s)X = Y \) for some \( Y \) in \( \mathbb{R}^{m-1} \), \( M(r)M(s)X = M(r)Y = Z_y(r) \) each \( r \in [0,t] \) where \( Z_y(0) = Y \) and \( Z'_y = QZ \). Let \( h(r) = M(r+s)X = \)
$Z_x(r+s)$ where $Z'_x = QZ_x$. Then $h(0) = M(0+s)X = Y = Z'_y(0)$, $h' = Qh$, and by uniqueness $h(r) = M(r+s)X = Z'_y(r) = M(r)M(s)X$.

Theorem 2. Let $r > 0$ and $w = |Q|$. Then $|M(r)| \leq e^{wr}$.

Proof. Let $X \in \mathbb{R}^{m-1}$ so that $||X|| = 1$. Then $M(r)X = Z_x(r)$ where $Z(0) = X$ and $Z'_x = QZ_x$. Since $Z'_x(r) = QZ_x(r)$ then

$f^rZ'_x = f^rQZ_x$, $Z_x(r) - Z_x(0) = Q\int_0^r Z'_x$ and $Z_x(r) = Z_x(0) + Q\int_0^r Z'_x$.

Let $g(r) = ||M(r)X|| = ||Z_x(r)||$. So $g(r) = ||Z_x(0) + Q\int_0^r Z'_x|| \leq ||Z_x(0)|| + ||Q\int_0^r Z'_x|| \leq ||X|| + |Q||\int_0^r Z'_x|| = 1 + w||\int_0^r Z'_x|| \leq 1 + w f^r g$.

Define $g_n(r) = g(r) \leq 1 + w f^r g$, $n = 0, 1, 2, \ldots$. Then

$g_{n+1}(r) \leq 1 + w f^r g_n$, $g_1(r) \leq 1 + w f^r g_0$, $g_2(r) \leq 1 + w f^r g_1 \leq 1 + w f^r (1 + w f_0^r s^1 d_0) d_1 = 1 + w f_0^r (w f_0^r s^1 g_0) ds_1 = 1 + w r + w^2 f_0^r f_0^r s^1 g_0 ds_1$. By induction $g_n(r) \leq 1 + w f_0^r g_{n-1} \leq 1 + w r + (w r)^2/2 + (w r)^3/3! \ldots + (w r)^{n-1}/(n-1)! + f_n(r)$, $n \in \mathbb{Z}^+$

where $f_n(r) = w \int_0^r (f^r s^1 g_0 ds_1) ds_2, \ldots ds_{n-1}$ and $f_0 = g_0$.

Note that $f_1(r) = w f_0^r g_0$, $f_2(r) = w f_0^r f_0^r s^1 g_0 ds_1 = w f^r w f_0^r s^1 g_0 ds_1 = w f^r f_1$ and by induction $f_{n+1}(r) = w f_0^r f_n$, $n = 1, 2, \ldots$. By Lemma 2, $\{f_n(r)\}_{n=1}^\infty = 0$.

Suppose $\varepsilon > 0$ and let $N$ denote a positive integer such that if $n \geq N$ $|f_n(r) - 0| = f_n(r) < \varepsilon$. Then $||M(r)X|| = g(r) = g_n(r) \leq 1 + w r + (w r)^2/2! + \ldots + (w r)^{n-1}/(n-1)! + f_n(r) < e^{wr} + \varepsilon$. 

Then \( ||M(r)X|| = g(r) = g_n(r) \leq 1 + wr + (wr)^2/2! + \ldots + (wr)^{n-1}/(n-1)! + R_n(r) < e^{wr} + \varepsilon \). Since \( ||X|| = 1 \) it follows that \( |M(r)| < e^{wr}, \ r > 0 \).

**Theorem 3.** \( ||M(r)-(I+rQ)|| \leq ((wr)^2/2)e^{wr}, \ r > 0 \).

**Proof.** Since \( M' (r) = QM(r) \) (Lemma 4) and \( M(0) = I \) (see definition 3), then \( f_0^r M' = f_0^r QM, M(r) - M(0) = f_0^r QM, \) and \( M(r)-I = f_0^r QM \). If follows that \( M(r)-I-rQ = f_0^r QM - f_0^r Q = f_0^r QM - f_0^r Q - f_0^r s^2 ds + f_0^r s^2 ds \) (where \( Q^2 \) is \( Q \) composed with \( Q \)) = \( f_0^r (QM(s) - Q - s Q^2) ds + f_0^r s Q^2 ds = f_0^r Q(M(s) - I - s Q) ds + f_0^r Q s Q^2 ds \). Let \( h(r) = M(r) - (I+rQ) \) = \( (rQ)^2/2 + Q f_0^r (M(s) - (I+sQ)) ds \). Let \( g(r) = |h(r)| \leq (r^2|Q|^2)/2 + |Q| f_0^r |h| \)

Now, let \( g_n(r) = g(r), \ n = 0,1,2,\ldots \). Then

\[ g_1(r) = (wr)^2/2 + w f_0^r g_0, \ g_2(r) = (wr)^2/2 + w f_0^r g_1 = (wr)^2/2 + w f_0^r ((ws_1)^2/2 + w f_0^r s_1 g_0) ds_1 = (wr)^2/2 + w w^2/2 f_0^r s_1^2 ds_1 + w f_0^r (w f_0^r s_1 g_0) ds_1 = (wr)^2/2 + (w^3/2)(r^3/3) + w^2 f_0^r f_0^r s_1^2 g_0 ds_1 \]

\[ (wr)^2/2! + (wr)^3/3! + w^2 f_0^r f_0^r s_1 g_0 ds_1, \] and \( g_n(r) = g(r) = (wr)^2/2! + \ldots + (wr)^{n+1}/(n+1)! + w f_0^r f_0^r s_1 \ldots (f_0^r s_1 g_0) ds_1 \ldots ds_{n-1} \).

Let \( y_0 = g_0 \) and \( y_{n+1}(r) = w f_0^r y_n \ n = 0,1,2,\ldots \). By Lemma 2 \( \{y_n(r)\}_{n=1}^\infty \to 0 \). Using induction we observe that \( y_n(r) = w^n f_0^r (f_0^r s_{n-1} \ldots (f_0^r s_1 g_0) ds_1 \ldots ds_{n-1} \).

Let \( \epsilon > 0 \) and \( N \) be a positive integer so that if \( n \geq N \) then

\[ |y_n(r) - 0| = y_n(r) < \epsilon \] and suppose \( n \geq N \).
Then \( g_n(r) = g(r) = (\sum_{k=2}^{n+1} \frac{(wr)^k}{k!}) + y_n(r) < (\sum_{k=2}^{\infty} \frac{(wr)^k}{k!}) + \varepsilon = \frac{(wr)^2}{2} \left( \frac{1}{3} + \frac{(wr)^2}{3} \cdot \frac{4}{5} + \cdots \right) + \varepsilon \leq \frac{(wr)^2}{2} e^{wr} + \varepsilon. \) So

\[
|M(r)-(I+rQ)| = |h(r)| = g(r) \leq \frac{(wr)^2}{2} e^{wr}.
\]

Lemma 4. \( M'(r) = Q M(r) \) \( r > 0. \)

Indication of proof. \( M \) is associated with an \((m-1) \times (m-1)\) function-valued matrix each element of which is differentiable on \([0, t]\).

Furthermore, the \(i\)th column of the matrix associated with \(M(r)\) is obtained by evaluating \(M(r)\) at the \(i\)th basis element: \(M(r)c_i\). Given \(Y \in \mathbb{R}^{m-1}, Z_y(r) = M(r)Y,\) and \(Z'_y(r) = QZ_y(r)\) (refer to definition 3), we have \(\frac{Z_y(r)-Z_y(s)}{r-s} + Z'_y(r)\) as \(s \to r;\) therefore \(\frac{M(r)Y - M(s)Y}{r-s} = \frac{M(r) - M(s)}{r-s} Y + Z'_y(r) = QZ_y(r).\) Hence \(QM(r)Y = M'(r)Y\) for all \(Y\) and so \(M'(r) = QM(r).\)

The following highly useful theorem is used as a lemma for Theorems 4 and 8 in this paper.

Lemma 5. (Difference of products). Suppose \(R\) is a ring with identity (not necessarily commutative), \(n \in \mathbb{Z}^+\) and each of \(a_1, a_2, \ldots, a_n, b_1, b_2, \ldots, b_n\) is an element in \(R.\) Then

\[(a_1 a_2 \cdots a_n) - (b_1 b_2 \cdots b_n) = \sum_{k=1}^{n} (a_1 a_2 \cdots a_{k-1}) (a_k - b_k)(b_{k+1} \cdots b_n)\]

where the first factor is 1 when \(k = 1\) and the third factor is 1 when \(k = n.\)

Indication of proof. Expanding the sum \(\sum_{k=1}^{n} (a_1 \cdots a_{k-1}) (a_k - b_k)(b_{k+1} \cdots b_n),\) each product of three factors becomes a pair of terms with alternating signs. The
first term (with positive sign) of each pair cancels with the second term (which has negative sign) of the subsequent pair. After cancellation the second term of the first pair and the first term of the last (nth) pair remain: 

\[-(b_1b_2\cdots b_n) + (a_1a_2\cdots a_n)\]

**Theorem 4.** Let \( t > 0, \ w = |Q|, \) and \( \varepsilon > 0. \) Then there is a positive integer \( N \) so that if \( n \geq N, \ \text{M}(t) - (I + (t/n)Q)^n 1 < \varepsilon. \)

**Proof.** Choose \( N \) so that \( (1/N)^{(1/2)(w^t)} < c, \) let \( n > N, \) and \( \delta = t/n: \)

\[
|M(t) - (I + \delta Q)^n| = |M(t)_{n+1} - t_n| \cdots \cdot M(t_{2} - t_1) - (I + \delta Q)^n|
\]

\[
= |M(t/n)^n - (I + \delta Q)^n| \quad \text{where} \quad t_\delta = (k-1)t/n, \ k = 1, 2, \ldots, n+1 \quad \text{and}
\]

hence \( (t_{k+1} - t_k) = t/n = \delta. \) By Lemma 5 \( |M(\delta)_{n} - (I + \delta Q)^n| = \)

\[
|\sum_{k=1}^{n} M(\delta)_{k+1} - M(\delta)_{k} - (I + \delta Q)^{n-k} | \leq \sum_{k=1}^{n} |M(\delta)_{k+1} - M(\delta)_{k} - (I + \delta Q)^{n-k}|
\]

\[
(1 + \delta w)^{n-k} \leq \sum_{k=1}^{n} (e^{w\delta})_{k+1} \left( (\frac{w\delta}{2})^{k} e^{w\delta} \right) (1 + \delta w)^{n-k} \quad \text{(Theorems 2 and 3)} \leq \sum_{k=1}^{n} (e^{w\delta})_{k+1} \left( (\frac{w\delta}{2})^{k} e^{w\delta} \right) (e^{w\delta})_{n-k} = \sum_{k=1}^{n} (e^{w\delta})_{n} (1/2) (w\delta)^{2}
\]

\[
= (1/2) (w\delta)^{2} \sum_{k=1}^{n} e^{wt} = (1/2) (w t/n)^2 n \ e^{wt} = (1/n)(1/2) (wt)^2 e^{wt} < \varepsilon.
\]

**Conclusion:** \( \lim_{n \to \infty} (I + (t/n)Q)^{n} Y_1 = M(t)Y_1 = f(t) = Y_{n+1}. \)
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CHAPTER III

AN IMPLICIT METHOD

In order to show that the first (and simpler) of the two implicit methods described in Chapter I "works"; that is, that \((I-\delta Q)^{-1} + M(t)\), we shall first show that \((I-\delta Q)^{-1}\) exists and furthermore, \(|I-\delta Q|^{-1} \leq 1\).

Here we refer to definition 2 (Chapter II) and to the notation in Chapter I. Recall that \(-Q = A^*A\) where \(A^*\) (called a transpose) represents the square matrix such that the \(i\)th column of \(A\) is the \(i\)th row of \(A^*\). We shall use some facts from linear algebra. See Chapter II(1).

**Fact 3.** If \(A\) represents an \(m \times m\) matrix and each of \(X\) and \(Y\) is in \(R^m\) note that \(AX,Y = X,A^*Y\) (where \(X,Y = \sum_{i=1}^{m} x_i y_i\)).

**Fact 4.** Suppose \(A\) is a linear transformation from \(R^m\) to \(R^m\). Then the following are equivalent:

1) \(AX = 0\) only if \(X = 0\).
2) The range of \(A\) is all of \(R^m\).
3) \(A\) has an inverse.

**Lemma 6.** Let \(\delta > 0\), \(A\) represent an \(m \times m\) matrix, and \(X \in R^m\). Then \(\|(I+\delta A^*A)X\| \geq \|X\|\).
Proof. Let $Y = AX$. Then

$$\| (I + \delta A^* A)X \|^2 = \langle (I + \delta A^* A)X, (I + \delta A^* A)X \rangle = \langle IX + \delta A^* AX, IX + \delta A^* AX \rangle = \langle X + \delta A^* Y, X + \delta A^* Y \rangle = \langle X, X \rangle + 2 \langle X, \delta A^* Y \rangle + \delta^2 \langle A^* Y, A^* Y \rangle \geq \langle X, X \rangle + 2 \delta \langle X, A^* Y \rangle + \delta^2 \langle A^* Y, A^* Y \rangle.$$ (Fact 3)

$$= \langle X, X \rangle + \delta \langle Y, Y \rangle + \delta^2 \langle A^* Y, A^* Y \rangle \geq \langle X, X \rangle = \|X\|^2; \text{ hence}$$

$$\| (I + \delta A^* A)X \| \geq \|X\|.$$ 

Lemma 7. $(I + \delta A^* A)$ is invertible, $\delta > 0$.

Proof. If $(I + \delta A^* A)X = 0$ it follows, using Lemma 6, that

$$0 \leq \|X\| \leq \|(I + \delta A^* A)X\| = \|0\| = 0; \text{ hence } X = 0. \text{ Therefore } (I + \delta A^* A)^{-1} \text{ exists (Fact 4).}$$

Lemma 8. $|I + \delta A^* A|^{-1} \leq 1$.

Proof. Since $\|(I + \delta A^* A)X\| \geq \|X\|$ it follows that $|I + \delta A^* A| \geq 1$. Suppose $Y \in \mathbb{R}^m$ and let $X = (I + \delta A^* A)^{-1}Y$. Then

$$\|Y\| = \|(I + \delta A^* A)X\| \geq \|X\| \text{ (Lemma 6). So } \|Y\| \geq \|(I + \delta A^* A)^{-1} (I + \delta A^* A)X\| = \|(I + \delta A^* A)^{-1}Y\| \text{. Since we have } \|(I + \delta A^* A)^{-1}Y\| \leq \|Y\| \text{ for an arbitrary vector } Y \text{ then } |(I + \delta A^* A)^{-1}| \leq 1.$$

Theorem 5. For $r > 0$, $|M(r) - I| \leq e^{wr} - 1$.

Proof. From $M(r) = QM(r)$ we have $M(r) - M(0) = \int_0^r QM$; therefore

$$|M(r) - I| = \left| \int_0^r QM(s) \right| ds \leq \int_0^r |Q| \left| M(s) \right| ds \leq \int_0^r w |M(s)| ds \leq \int_0^r we^{ws} ds \text{ (Theorem 2)} = e^{wr} - 1.$$

Theorem 6. $|M(r) - (I + rQM(r))| \leq (3/2)(wr)^2 e^{wr}$, $r > 0$.

Proof. $|M(r) - (I + rQM(r))| = |M(r) - I - rQ + rQ - rQM(r)| \leq ((wr)^2/2)e^{wr} + rw(e^{wr}) - 1 \leq (wr)^2/2 e^{wr} + wr(e^{wr} - 1) = (3/2)(wr)^2 e^{wr}$. 

[we refer to Theorems 3 and 5 and to the fact that $e^x - 1 \leq x e^x$, $x > 0$ (look at series)],

Theorem 7. $|M(r) - (I - rQ)^{-1}| \leq (3/2)(w)2 e^{wt}$.

Proof. $|M(r) - (I - rQ)^{-1}| = |(I - rQ)^{-1}(I - rQ)M(r) - (I - rQ)^{-1}| = |(I - rQ)^{-1}((I - rQ)M(r) - I)| \leq |(I - rQ)^{-1}| |(I - rQ)M(r) - I| \leq 1. |M(r) - I - rQM(r)| \leq (3/2)(w)2 e^{wt}$ (Lemma 8, Theorem 6).

Theorem 8. Suppose $t > 0$ and $\epsilon > 0$. There is a positive integer $N$ so that if $n \geq N$, $|M(t) - (I - (t/n)Q)^{-n}| \leq \epsilon$.

Proof. Let $N \in \mathbb{Z}^+$ so that $(1/N)(3/2)(w)2 e^{wt} < \epsilon$, $n \geq N$, and $\delta = t/n$. Then $|M(t) - (I - (t/n)Q)^{-n}| = |M(t_{n+1} - t_n) \cdots M(t_{t_1} - (I - \delta Q)^{-1})|$

$\leq \sum_{k=1}^{n} |M(\delta)^k - (I - \delta Q)^{-k}||I - (I - \delta Q)^{-1}|(3/2)(w)2 e^{w\delta} \cdot 1$ (Theorems 2 and 7, Lemma 8) = $\sum_{k=1}^{n} (e^{w\delta})^k(3/2)(w)2 e^{w\delta}$

$\leq \sum_{k=1}^{n} (e^{w\delta})^k(3/2)(w)2 e^{w\delta} = \sum_{k=1}^{n} e^{wt}(3/2)(w)2 = n w^2(t/n)^2(3/2)e^{wt} = (1/n)(3/2)(w)2 e^{wt} < \epsilon$. Conclusion. $(I - (t/n)Q)^{-n} \rightarrow M(t)$ as $n \rightarrow \infty$. 
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CHAPTER IV

CRANK-NICOLSON METHOD

In this chapter, we wish to demonstrate \((I-(t/2n)Q))^{-n}\) \((I+(t/2n)Q)^n\) \(M(t)\) as \(n \to \infty\). We shall first show that 
\[|M(t)| \leq 1 \text{ for } t > 0.\]
We have already seen (Chapter II) that 
\[|M(r)| \leq e^{|r|t} \text{ for } r \geq 0.\]
Now that we have Theorem 8 at our disposal, we are in position to get a better bound on \(|M(t)|\).

Theorem 9. \(|M(t)| \leq 1 \quad t > 0.\)

Proof. \((I-(t/2n)Q))^{-n} \to M(t)\) as \(n \to \infty\) (Theorem 8) and 
\[|(I-(t/2n)Q)^{-1}| \leq 1 \text{ according to Lemma 8, so } |(I-(t/2n)Q)^{-n}| \leq 1 \text{ each } n; \]
therefore \(\lim_{n \to \infty} |(I-(t/2n)Q)^{-n}| \leq 1.\)
Given \(Y \in \mathbb{R}^{m-1}\)
\[||M(t)Y|| = ||\lim_{n \to \infty} (I-(t/2n)Q)^{-n}Y|| = \lim_{n \to \infty} ||(I-(t/2n)Q)^{-n}Y|| \leq \]
\[\lim_{n \to \infty} ||(I-(t/2n)Q)^{-n}|| \cdot ||Y|| \leq 1. \quad ||Y|| = ||Y||. \quad \text{Since } ||M(t)Y|| \leq M(t)||Y||, \text{ it follows that } |M(t)| \leq 1.\]

Theorem 10. Let \(t > 0.\) If \(\varepsilon > 0\) there is a positive integer \(N\) so that if \(n \geq N \quad |M(t)-((I-(t/2n)Q)^{-1}(I+(t/2n)Q))^n| < \varepsilon.\)

Proof. Due to commutativity (see page 12) we note that 
\([(I-(t/2n)Q)^{-1}(I+(t/2n)Q))^n = (I-(t/2n)Q)^{-1}(I+(t/2n)Q))^n.\]
Let \(L = e^{|t|t/2}\), a bound on \(|(I+(t/2n)Q)^n|\) for all positive integers \(n\), let \(\varepsilon > 0\), and let \(N \in \mathbb{Z}^+\) so that
1. \( (1/N)(3/2)(wt/2)^2 e^{wt/2} < \varepsilon/(2L) \) and \\
2. \( (1/N)(1/2)(wt/2)^2 e^{wt/2} < \varepsilon/2. \)

Then if \( n \geq N \), following from Theorems 8 and 4, it is the case that 
\[ |M(t/2)-(I-(t/2n)Q)^{-n}| < \varepsilon/(2L) \] and 
\[ |M(t/2)-(I+(t/2n)Q)^n| < \varepsilon/2. \]

Let \( \delta/2 = t/2n \). Then 
\[ |M(t)-(I-(\delta/2)Q)^{-n}(I+(\delta/2)Q)^n| \leq \\
|M(t/2) M(t/2) - M(t/2)(I+(\delta/2)Q)^n| + |M(t/2)(I+(\delta/2)Q)^n - (I-(\delta/2)Q)^{-n}(I+(\delta/2)Q)^n| \leq |M(t/2)| |M(t/2)-(I+(\delta/2)Q)^n| + \\
|M(t/2)-(I-(\delta/2)Q)^{-n}| |(I+(\delta/2)Q)^n| < 1 \cdot \varepsilon/2 + \varepsilon |(2L)e^{wt/2}|

(Theorem 9) = \varepsilon/2 + \varepsilon/(2L) \cdot L = \varepsilon.
CHAPTER V

CONCLUSIONS AND FUTURE PLANS

It is hoped that some insight may be gained from the preceding analysis of but a few computational schemes. Many other algorithms are available, some of which have already been pursued by this author. Not included in this paper, for example, is the explicit quadratic method, giving second order accuracy. Another scheme of at least theoretical interest, is one of successive approximations -- fitting in with the existence theorem (Theorem 1). Using a left end-point linear method, convergence is achieved to the same approximating solution as in the explicit linear case. Since a system of initial functions over $[0,t]$ is "assumed", both right end-point and mid-point values for approximating the integral are available. One of these choices might give somewhat better than first order accuracy for some types of problems. If so, the idea might prove useful in non-linear cases.

A combination of the explicit linear and the successive approximations schemes is currently in use. Here second order accuracy that generalizes to non-linear problems can be obtained by using a "successive" approximations algorithm twice to get estimates at the first intermediary time step. Then the process is continued.
Another idea to consider is simply averaging the explicit results (which are under-approximations) with the first implicit method results (over-approximations). There may be occasions when this scheme could serve in place of the somewhat more elaborate Crank-Nicolson method.

An investigation of machine (round-off) error is planned. And also further work on getting better bounds on error estimates (theoretically).

Also on the agenda is to let $m$, the number of space subdivisions, vary, as well as the number $(n)$ of time subintervals -- then show convergence to the actual solution.

A study of other types of equations, some requiring much different solving techniques, is planned. In the meantime the author is completing work on adapting the codes in this paper to the more general differential equation:

$$u_1(t,x) = v_2(t,x),$$

where $v(t,x) = g(x) u_2(t,x)$, $g$ continuous on $[0,1]$. 
APPENDIX

Three FORTRAN codes are included here. The first is the explicit linear method, the second is the "right-sided" implicit method, also linear, and the third is the Crank-Nicolson, which is a central difference implicit method.

Following the programs are some tables with numerical results. The first three numbers represent the number of space and time subintervals and the ratio \( \alpha = \delta/(Dx)^2 \). The codes allow for different space and time interval lengths as well as changes in the number of subdivisions of each. The initial value function and the boundary values may also be changed.

The program executions that follow the codes represent only cases where the boundary values are 0, the space interval is \([0,1]\) and the time interval is \([0,1]\). Two initial condition functions are considered: \( h(x) = \sin \pi x \) and \( h(x) = x(1-x) \). The second initial condition function does not give rise to a closed form answer so no comparison is made with an "actual solution."

The left column of each table represents the times and the top row the points in space (i.e. positions along the rod) that go along with the numerical estimate.

Notice the symmetry along the space interval generated by the initial conditions. Notice also the instability of the
explicit method when the ratio $\delta/(Dx)^2$ is 1. This problem does not occur when either of the implicit schemes is used.

The Crank-Nicolson code compares the first IMPLICIT method, the CN, and the ACTUAL solution. Observe the greater accuracy of the Crank-Nicolson.

Work on the pages to follow was done on the Dec-System 20 at Texas Women's University. All tables are numerical results for the heat equation using zero boundary values.
C: HELI=HEAT EQUATION, LINEAR (EXPLICIT METHOD)

COMMON RDX2, PI
DIMENSION Y(11,2), X(11)
PI=3.14159265
DI=1.
NS=5
LS=1
DX=DI/FLOAT(NS)
RDX=1./DX
RDX2=RDX**2
NSP1=NS+1
M=1
MP1=M+1
X1=0.
T1=0.
DO 10 J=1,NSP1
  Y(J,1)=H((J-1)*DX)
D=1.
N=50
LN=10
DT=D/FLOAT(N)
ALFA=DT*RDX2
WRITE(5,3)
3 FORMAT('O',12X,'EXPLICIT LINEAR METHOD')
WRITE(5,5)
5 FORMAT('OvX,'INITIAL FUNCTION: SIN(PI*X)')
WRITE(5,7)NS,N,ALFA
7 FORMAT('O',I4,4X,I6,5X,F6.2)
DO 8 J=2,NS
  X(J)=X1+(J-1)*DX
  WRITE(5,2) (X(J),J=MP1,NS,LS)
2 FORMAT('O',3X,6(F11.2))
WRITE(5,4)T1,(Y(J,1),J=MP1,NS,LS)
4 FORMAT('O',F6.2,6(F11.5))
DO 11 I=1,N
  T2=T1+DT
DO 12 J=2,NS
  QY=F(T1,Y(J-1,1),Y(J,1),Y(J+1,1))
  Y(J,2)=Y(J,1)+DT*QY
12 CONTINUE
T1=T2
DO 13 J=2,NS
  Y(J,1)=Y(J,2)
  IF (I/LN*LN,LT,1) GOTO 11
WRITE(5,6)T2,(Y(J,2), J=2,NS,LS)
6 FORMAT('O',F6.2,6(F11.5))
11 CONTINUE
STOP
END
FUNCTION H(X)
COMMON RDX2, PI
H=SIN(PI*X)
RETURN
END
FUNCTION F(Q,R,S,T)
COMMON RDX2, PI
F=RDX2*(T-2.*S+R)
RETURN
END
C: AN IMPLICIT METHOD FOR HEAT EQUATION

COMMON PI
DIMENSION X(101),A(101),B(101),Y(101),U(101),Z(101)
PI=3.14159265
Q=-PI**2
DI=1.
NS=5
LS=1
M=1
MP1=M+1
LSP1=LS+1
D=1.
N=25
LN=5
NSP1=NS+1
NSP2=NS+2
NSM1=NS-1
NP1=N+1
DX=DI/FLOAT(NS)
RDX=1./DX
RDX2=RDX**2
DT=D/FLOAT(N)
T=0.
X1=0.
ALFA=D*RDX2
BETA=2.*ALFA+1.
WRITE(5,2)
2 FORMAT('0',11X,'RIGHT-SIDED IMPLICIT METHOD')
WRITE(5,5)
5 FORMAT('INITIAL FUNCTION: SIN(PI*X)')
WRITE(5,3) NS,N,ALFA
3 FORMAT('0',I4,4X,I6,5X,F6.2)
DO 30 K=1,NSP1
   Y(K)=H((K-1)*DX)
   U(1)=0.
   U(NSP1)=0.
   A(K)=-ALFA
   B(K)=BETA
30 CONTINUE
DO 20 K=2,NS
   X(K)=X1+(K-1)*DX
20 CONTINUE
WRITE(5,7) (X(K),K=MP1,NS,LS)
7 FORMAT('0',3X,6(F11.2))
WRITE(5,4) T1*(Y(K),K=MP1,NS,LS)
4 FORMAT('0',F6.2,6(F11.5))
DO 100 J=2,NP1
    T2=T1+DT
25  DO 40 K=3,NS
    Y(K)=Y(K)-(A(K)/B(K-1))*Y(K-1)
    B(K)=B(K)-(A(K)/B(K-1))*A(K-1)
40  CONTINUE
   DO 50 K=1,NSM1
   U(NSP1-K)=(Y(NSP1-K)-A(NSP1-K)*U(NSP2-K))/B(NSP1-K)
   CONTINUE
   IF((J-1)/LN*LN.EQ.(J-1)) WRITE(5,6) T2, (U(K),K=MP1,NS,LS)
6  FORMAT( ' ', 'F6.2,6(F11.5)')
   DO 60 K=2,NS
   B(K)=BETA
   Y(K)=U(K)
   Z(K)=EXP(Q*T2)*H((K-1)*DX)
60  CONTINUE
   IF((J-1)/LN*LN.EQ.(J-1)) WRITE(5,10) (Z(K),K=MP1,NS,LS)
10  FORMAT( ' ', 'ACTUAL', '6(F11.5)')
   T1=T2
100 CONTINUE
STOP
END
FUNCTION H(X)
COMMON PI
H=SIN(PI*X)
RETURN
END
C: IMPLICIT & CRANK-NICOLSON FOR HEAT EQUATION

COMMON PI
DIMENSION X(101), C(101), D(101), F1(101), F2(101), Z(101)
DIMENSION Y1(101), Y2(101), A(101), B(101)
DIMENSION V(101)
PI=3.14159265
Q=-(PI**2)
DI=1.
NS=20
LS=4
LSP1=LS+1
M=2
MP1=M+1
DJ=1.
N=200
LN=20
NSP1=NS+1
NSP2=NS+2
NSM1=NS-1
NP1=N+1
DX=DI/FLOAT(NS)
RDX=1./DX
RDX2=RDX**2
DT=DJ/FLOAT(N)
T1=0.
X1=0.
ALFA=DT*RDX2
BETA =1.*+2.*ALFA
WRITE(5,3)
3 FORMAT(’O’,13X,’IMPLICIT AND CRANK NICOLSON METHODS’)
WRITE(5, 14)
14 FORMAT(’ ’,17X,’INITIAL FUNCTION: SIN(PI*X)’)
DO 30 K=1,NSP1
   Y1(K)=H((K-1)*DX)
   F1(K)=Y1(K)
   Y2(1)=0.
   F2(1)=0.
   Y2(NSP1)=0.
   F2(NSP1)=0.
   A(K)=-ALFA
   B(K)=BETA
   C(K)=-ALFA/2.
   D(K)=1.+ALFA
30 CONTINUE
WRITE (5,2) NS,N,ALFA
2 FORMAT(’O’,I4,4X,I6,5X,F6,2)
DO 5 K=2,NS
   X(K)=X1+(K-1)*DX
5
WRITE (5,7) (X(K), K=MP1,NS,LS)
7
FORMAT ('0',3X,6(F11.2))
WRITE(5,4)T1,(Y1(K),K=MP1,NS,LS)
4
FORMAT(' ',F6,2,6(F11.5))
DO 100 J=2,MP1
   T2=T1+DT
100
DO 20 K=2,NS
   V(K)=F1(K)+(ALFA/2.)*(F1(K-1)-2.*F1(K)+F1(K+1))
20
CONTINUE
IF((J-1)/LN*LN.LT.(J-1))GOTO 25
25
DO 40 K=3,NS
   Y1(K)=Y1(K)-(A(K)/B(K-1))*Y1(K-1)
   V(K)=V(K)-(C(K)/D(K-1))*V(K-1)
   B(K)=B(K)-(A(K)/B(K-1))*A(K-1)
   D(K)=D(K)-(C(K)/D(K-1))*C(K-1)
40
CONTINUE
DO 50 K=1,NSM1
   Y2(NSP1-K)=(Y1(NSP1-K)-A(NSP1-K)*Y2(NSP2-K))/B(NSP1-K)
   F2(NSP1-K)=(V(NSP1-K)-C(NSP1-K)*F2(NSP2-K))/D(NSP1-K)
50
CONTINUE
IF((J-1)/LN*LN.LT.(J-1))GOTO 9
9
WRITE(5,12)T2,(Y2(K),K=NSM1,NS,LS)
12
FORMAT(' ',F6,2,6(F11.5))
WRITE(5,8)F2(K),K=MP1,NS,LS)
8
FORMAT(' ',CN,:),2X,6(F11.5))
9
DO 60 K=2,NS
   B(K)=BETA
   D(K)=ALFA
   Y1(K)=Y2(K)
   F1(K)=F2(K)
   Z(K)=EXP(Q*T2)*H((K-1)*DX)
60
CONTINUE
IF((J-1)/LN*LN.LT.(J-1))GOTO 11
WRITE(5,10)(Z(K),K=MP1,NS,LS)
10
FORMAT(' ',,'ACTUAL',6(F11.5))
11
T1=T2
100
CONTINUE
STOP
END
FUNCTION H(X)
COMMON PI
H=SIN(PI*X)
RETURN
END
**EXPLICIT LINEAR METHOD**

**INITIAL FUNCTION:** $\sin(\pi x)$

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**EXPLICIT LINEAR METHOD**

**INITIAL FUNCTION:** $\sin(\pi x)$

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**RIGHT-SIDED IMPLICIT METHOD**

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### IMPLICIT AND CRANK NICOLSON METHODS

**INITIAL FUNCTION: \( \sin(\pi x) \)**

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### Explicit Linear Method

**Initial Function:** \( x(1-x) \)

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**CPU time:** 0.26  
**Elapsed time:** 18.15

### Right-Sided Implicit Method

**Initial Function:** \( x(1-x) \)

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IMPLICIT AND CRANK NICOLSON METHODS
INITIAL FUNCTION: \((X*(1-X))\)

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CPU time 0.58  Elapsed time 1:03.16
BIBLIOGRAPHY


