c(

NUMERICAL SOLUTION OF LINEAR SECOND ORDER PARABOLIC EQUATIONS BY THE METHOD OF COLLOCATION WITH CUBIC SPLINES.

by

EUSEBIUS JACOBUS DOEDEL

B. Sc., University of British Columbia, 1971

A THESIS SUBMITTED IN PARTIAL FULFILMENT OF

THE REQUIREMENTS FOR THE DEGREE OF

MASTER OF SCIENCE

in the Department

of

Mathematics

We accept this thesis as conforming to the

required standard

THE UNIVERSITY OF BRITISH COLUMBIA

April, 1973

Department of Mathematics

The University of British Columbia
Vancouver 8, Canada

Date April, 1973.

Abstract

Collocation with cubic splines is used as a method for solving Linear second order parabolic partial differential equations. The collocation method is shown to be equivalent to a finite difference method that is consistent with the differential equation and stable in the sense of Von Neumann. Results of numerical computations are given, as well as an application of the method to a moving boundary problem for the heat equation.

Table of Contents

Acknowledgement

The author sincerely wishes to thank Professor James M. Varah for generous assistance during the course of the research.

He wishes to thank also the National Research Council of Canada for bursary support and the University of British Columbia for teaching assistanceships.

He is also thankful to Mrs. Magdalena Alemparte for the typing of his manuscript.

INTRODUCTION.

Collocation with piecewise polynomial functions has been developed as a method for solving two-point boundary value problems for ordinary differential equations by for example Russell and Shampine [13], and de Boor and Swartz [3].

Recently Douglas and Dupont [5] have proposed a collocation method with Hermite piecewise - cubic polynomials for solving non linear parabolic equations.

In this thesis an efficient method for solving linear second order parabolic equations by the method of collocation with cubic splines will be presented.

In Part I the collocation procedure will be introduced and shown to be equivalent to a finite difference schme that is second order accurate. With a uniform mesh and constant coefficients the finite difference scheme will be shown to be stable in the sense of Von Neumann, so that for this type of problem the solution of the finite difference equations converges to the solution of the continuous problem with second order accuracy.

The scheme has the advantage that like Keller's Box scheme [11] it does not require a uniform net. Approximate values of first and second derivatives at the net points can be obtained explicitly from the solution of the finite difference equations. Convergence of these to the corresponding derivatives of the continuous solution will not be shown; however, numerical computations seem to indicate that they are second order approximations, which is in agreement with the results obtained by Russell and Shampine. Finally the matrix equations resulting from the finite difference equations involve only tridiagonal matrices that are of the same dimension as those of the corresponding Crank Nicholson scheme.

In Part II a number of problems will be solved using the scheme and the results will be compared to those obtained by the Box scheme and the Crank Nicholson scheme.

In Part III we shall indicate how the scheme can be used to obtain an approximate solution to a Stefan problem and some numerical results will be given.

It is not neccessary to restrict to cubic splines in the collocation scheme. Good results have been obtained using Hermite piece-wise quintic polynomials for example.

The cubic spline collocation scheme wins, however, as far as simplicity is concerned.

PART I.

I.1 Description of the Collocation Scheme.

Consider the linear second order parabolic P. D. E.

$$(py)_t = y_{xx} + qy_x + ry + f \qquad (0 \leqslant x \leqslant 1)$$
$$(0 \leqslant t \leqslant T)$$

with p, q, r and f functions of x and t.

Upon setting

$$z = e^{\frac{1}{2}\int^x q\,dx} . \hat{y}$$

we find that satisfies

$$(pz)_t = z_{xx} + (r - q_x/2 - q^2/4 + (p/2)\int^x q_t\,dx)\,z + e^{\frac{1}{2}\int^x q\,dx} . f$$

We assume that the indefinite integrals $\int^x q\,dx$ and $\int^x q_t\,dx$ can be evaluated, so we may restrict our attention to equations of the form

(1.1) $$(py)_t = y_{xx} + qy + f$$

subject to

(1.2) $$\begin{cases} y(x,0) = g(x) & (0 \leqslant x \leqslant 1) \\ \left.\begin{array}{l} y(0,t) = g_0(t) \\ y(1,t) = g_1(t) \end{array}\right\} & (0 \leqslant t \leqslant T) \end{cases}$$

We shall make the following assumptions: p,q and f are continuous functions of x and t, and p is three times continuously differentiable with respect to t in $R(T) = [0,1] \times [0,T]$.

The equation (1.1) must be parabolic in the sense of Petrowski, i.e.

$$p(x,t) \geqq p_* > 0 \text{ for } (x,t) \in R(T)$$

Finally we assume that there is a unique solution to the differential equation (1.1) subject to the initial and boundary conditions (1.2), and that this solution is three times continuously differentiable with respect to t and four times continuously differentiable with respect to x.

On the rectanble R(T) place a net $R_h(T)$ such that

$$x_0 = 0 \qquad x_J = 1 \qquad t_0 = 0 \qquad t_N = T$$

with netspacings

$$h_j = x_j - x_{j-1} \qquad (1 \leq j \leq J)$$

$$k_n = t_n - t_{n-1} \qquad (1 \leq n \leq N)$$

We shall use the following notation:

For functions defined on $R_h(T)$:

$$\varphi_j^n = \varphi(x_j, t_n)$$

For functions defined on $R(T)$:

$$\varphi_j^n = \varphi(x_j, t_n)$$

$$(\varphi_z)_j^n = \varphi_z(x_j, t_n)$$ where the subscript z represents a first or higher order derivative with respect to x or t.

$$\varphi_j^{n-\frac{1}{2}} = \varphi(x_j, t_n - k_n/2)$$

For functions defined on $[0,1] \times [t_n]$:

$$\varphi_j^n = \varphi(x_j, t_n)$$

$$\varphi^n = \varphi(x, t_n)$$

$$(\varphi_z)_j^n = \varphi_z(x_j, t_n)$$

$$(\varphi_z)^n = \varphi_z(x, t_n)$$

Given a partition $0 = x_0 < x_1 < \ldots . < x_J = 1$ of the interval $[0,1]$, a <u>spline</u> of degree m defined on

$[0,1]$ is a function $S \in C^{m-1}[0,1]$ that is given by some polynomial of degree m or less in each subinterval $[x_j, x_{j+1}]$ $(0 \leqslant j \leqslant J-1)$. The points $\{x_j\}_{j=0}^{J}$ are called the <u>knots or joints</u> of the spline function. In particular if S is a cubic spline defined on the unit interval then $S \in C^2[0,1]$ and in each subinterval $[x_j, x_{j+1}]$ $(0 \leqslant j \leqslant J-1)$ S is given by a polynomial of degree 3 or less. For an introduction to spline functions see for example [9]. A more rigorous treatment of splines can be found in [1].

The collocation procedure is now defined as follows. At each time level t_n $(1 \leqslant n \leqslant N)$ we look for an approximate solution S^n to the problem (1.1, 1.2) satisfying

(1.3) S^n is a cubic spline defined on $[0,1] \times [t_n]$

(1.4) The boundary conditions:

$$S_0^n = g_0(t_n)$$

$$S_J^n = g_1(t_n)$$

(1.5) The collocation conditions:

$$\frac{p_j^n S_j^n - p_j^{n-1} S_j^{n-1}}{k_n} = \frac{1}{2}\left\{ (S_{xx})_j^n + q_j^n S_j^n + f_j^n + (S_{xx})_j^{n-1} + q_j^{n-1} S_j^{n-1} + f_j^{n-1} \right\}$$

$$(0 \leqslant j \leqslant J)$$

Where we let S^0 be the cubic spline interpolant of the initial data g(x), (i.e. $S_j^0 = g(x_j) \quad (0 \leq j \leq J)$) satisfying the endpoint conditions:

$$(S_{xx})_0^0 = g_{xx}(0)$$

and

$$(S_{xx})_J^0 = g_{xx}(1)$$

In the special case of the heat equation

$$y_t = y_{xx}$$

the collocation equation (1.5) becomes

$$\frac{S_j^n - S_j^{n-1}}{k_n} = \frac{1}{2}\left\{ (S_{xx})_j^n + (S_{xx})_j^{n-1} \right\}$$

which resembles the Crank-Nicolson difference approximation

$$\frac{U_j^n - U_j^{n-1}}{k_n} = \frac{1}{2}\left\{ \frac{U_{j-1}^n - 2U_j^n + U_{j+1}^n}{h^2} + \frac{U_{j-1}^{n-1} - 2U_j^{n-1} + U_{j+1}^{n-1}}{h^2} \right\}.$$

Except that only the time variable has been discretized.

Usually the term collocation is meant to imply that the approximate solution S^n satisfies the differential equation exactly at a certain number of points. Because of the discretization in time this is actually not true for condition (1.5). However, we shall refer to condition (1.5) as the collocation condition.

I.2 The Finite Difference Scheme.

Since at each time level t_n the approximate solution S^n should be a cubic spline, it is determined uniquely by four coefficients per subinterval. That is we could represent S^n by

$$S^n(x) = q_{j,n}x^3 + b_{j,n}x^2 + c_{j,n}x + d_{j,n} \qquad (x_{j-1} \leqslant x \leqslant x_j)$$
$$(1 \leqslant j \leqslant J)$$

This would lead to $4J$ unknown coefficients per time level. These coefficients then could be obtained from the 2 boundary conditions (1.4), the $J + 1$ collocation conditions (1.5) and $3(J-1)$ continuity conditions. Such a procedure would give large systems to be solved, and is therefore not advisable.

Another approach would be to express S^n in terms of basis-functions having the property that a linear combination of these automatically satisfies the continuity conditions. Such basis-functions have been constructed, see for example [14] .

We shall not use either of the above methods; instead the collocation procedure will be shown to be equivalent to a finite difference method.

First this finite difference scheme will be stated and sufficient conditions will be given for the existence of a unique solution to the resulting matrix equation. In section I.3 we shall show that the finite difference scheme is consistent with the continuous problem. (1.1), and in section I.4 the scheme will be shown to be stable in the case of constant coefficients and a uniform net. The equivalence of the finite difference scheme and the collocation scheme will be settled by theorem 5.3 of section I.5. The difference scheme will then serve as the basis for the algorithm for solving the collocation scheme. The algorithm will be given in section I.6.

Consider the difference scheme defined by

$$
(2.1) \quad \begin{aligned}
L_h U_j^n &= 0 && (1 \leq j \leq J-1 \ , \ 1 \leq n \leq N) \\
U_0^n &= g_0(t_n) && (1 \leq n \leq N) \\
U_J^n &= g_1(t_n) && (1 \leq n \leq N) \\
U_j^0 &= g(x_j) && (0 \leq j \leq J)
\end{aligned}
$$

where

$$
\begin{aligned}
L_h U_j^n = {} & \frac{1}{3}\left\{ \frac{h_j}{h_j + h_{j+1}} \left(\frac{p_{j-1}^{n} U_{j-1}^{n} - p_{j-1}^{n-1} U_{j-1}^{n-1}}{k_n} \right) + 2 \left(\frac{p_j^n U_j^n - p_j^{n-1} U_j^{n-1}}{k_n} \right) \right. \\
& \left. + \frac{h_{j+1}}{h_j + h_{j+1}} \left(\frac{p_{j+1}^{n} U_{j+1}^{n} - p_{j+1}^{n-1} U_{j+1}^{n-1}}{k_n} \right) \right\} \\
& - \left\{ \frac{1}{2} \left[\frac{\dfrac{U_{j+1}^n - U_j^n}{h_{j+1}} - \dfrac{U_j^n - U_{j-1}^n}{h_j}}{\frac{1}{2}(h_j + h_{j+1})} + \frac{\dfrac{U_{j+1}^{n-1} - U_j^{n-1}}{h_{j+1}} - \dfrac{U_j^{n-1} - U_{j-1}^{n-1}}{h_j}}{\frac{1}{2}(h_j + h_{j+1})} \right] \right\} \\
& - \frac{1}{6}\left\{ \frac{h_j}{h_j + h_{j+1}} \left(q_{j-1}^n U_{j-1}^n + q_{j-1}^{n-1} U_{j-1}^{n-1} \right) + 2 \left(q_j^n U_j^n + q_j^{n-1} U_j^{n-1} \right) \right. \\
& \left. + \frac{h_{j+1}}{h_j + h_{j+1}} \left(q_{j+1}^n U_{j+1}^n - q_{j+1}^{n-1} U_{j+1}^{n-1} \right) \right\} \\
& - \frac{1}{6}\left\{ \frac{h_j}{h_j + h_{j+1}} \left(f_{j-1}^n + f_{j-1}^{n-1} \right) + 2 \left(f_j^n + f_j^{n-1} \right) + \frac{h_{j+1}}{h_j + h_{j+1}} \left(f_{j+1}^n + f_{j+1}^{n-1} \right) \right\}
\end{aligned}
$$

This difference scheme leads to matrix equations

$$(2.2) \qquad A^{(n)} \underline{U}^{(n)} = \underline{D}^{(n)} \qquad (1 \leqslant n \leqslant N)$$

where

$$A^{(n)} = \begin{vmatrix} 1 & & & & & & \\ a_1^n & b_1^n & c_1^n & & & O & \\ & a_2^n & b_2^n & c_2^n & & & \\ & & & \cdot & & & \\ & & & & \cdot & & \\ & & & & & \cdot & \\ & O & & & a_{J-1}^n & b_{J-1}^n & c_{J-1}^n \\ & & & & & & 1 \end{vmatrix}$$

$$\underline{U}^{(n)} = (U_0^n, U_1^n, \ldots\ldots, U_J^n)^T$$

and

$$\underline{D}^{(n)} = (d_0^n, d_1^n, \ldots\ldots, d_J^n)^T$$

with

$$(2.3) \quad a_j^n = \frac{h_j p_{j-1}^n}{3k_n} - \frac{1}{h_j} - \frac{h_j q_{j-1}^n}{6}$$

$$b_j^n = \frac{2(h_j + h_{j+1}) p_j^n}{3k_n} + \frac{1}{h_j} + \frac{1}{h_{j+1}} - \left(\frac{h_j + h_{j+1}}{3}\right) q_j^n$$

$$c_j^n = \frac{h_{j+1}\bar{p}_{j+1}^n}{3k_n} - \frac{1}{h_{j+1}} - \frac{h_{j+1}q_{j+1}^n}{6}$$

$$d_0^n = g_0(t_n)$$

$$d_J^n = g_1(t_n)$$

and

$$d_j^n = \left(\frac{h_j\bar{p}_{j-1}^{n-1}}{3k_n} + \frac{1}{h_j} + \frac{h_j q_{j-1}^{n-1}}{6}\right)U_{j-1}^{n-1}$$

$$+\left(\frac{2(h_j+h_{j+1})\bar{p}_j^{n-1}}{3k_n} - \frac{1}{h_j} - \frac{1}{h_{j+1}} + \frac{(h_j+h_{j+1})q_j^{n-1}}{3}\right)U_j^{n-1}$$

$$+\left(\frac{h_{j+1}\bar{p}_{j+1}^{n-1}}{3k_n} + \frac{1}{h_{j+1}} + \frac{h_{j+1}q_{j+1}^{n-1}}{6}\right)U_{j+1}^{n-1}$$

$$+\frac{1}{6}\left\{h_j(f_{j-1}^n + f_{j-1}^{n-1}) + 2(h_j + h_{j+1})(f_j^n + f_j^{n-1}) + h_{j+1}(f_{j+1}^n + f_{j+1}^{n-1})\right\}$$

Theorem 2.1

For each n ($1 \leqslant n \leqslant N$) there is a unique solution to the matrix equation (2.2) provided that

$$k_n < \frac{2\bar{p}^n_*}{q^{n*}}$$

and

$$\frac{h_j^2}{k_n} < \min \left\{ \frac{3}{\bar{p}^n_{j-1}} ; \frac{3}{\bar{p}^n_j} \right\} \qquad (1 \leqslant j \leqslant J) \tag{2.4}$$

where

$$q^{n*} = \max_j |q^n_j|$$

and

$$\bar{p}^n_* = \min_j (\bar{p}^n_j)$$

Proof.

It is sufficient to show that for each n ($1 \leqslant n \leqslant N$) the matrix $A^{(n)}$ of (2.2) is diagonally dominant, provided (2.4) holds. Specifically we want to show that

$$\left|b_j^n\right| - \left|a_j^n\right| - \left|c_j^n\right| > 0 \qquad (1\leqslant j\leqslant J-1\ ;\ 1\leqslant n\leqslant N)$$

Now

$$\left|b_j^n\right| \geqslant \frac{2(h_j+h_{j+1})}{3k_n} p_*^n + \frac{1}{h_j} + \frac{1}{h_{j+1}} - \frac{h_j+h_{j+1}}{3}\, q^{n*}$$

and

$$\left|a_j^n\right| \leqslant \left|\frac{h_j p_{j-1}^n}{3k_n} - \frac{1}{h_j}\right| + \frac{h_j}{6}\, q^{n*}$$

$$= \frac{1}{h_j} - \frac{h_j p_{j-1}^n}{3k_n} + \frac{h_j}{6}\, q^{n*} \qquad \left(\text{Since } \frac{h_j^2}{k_n} < \frac{3}{p_{j-1}^n}\right)$$

$$\leqslant \frac{1}{h_j} - \frac{h_j p_*^n}{3k_n} + \frac{h_j}{6}\, q^{n*}$$

Similarly

$$\left|c_j^n\right| \leqslant \frac{1}{h_{j+1}} - \frac{h_{j+1} p_*^n}{3k_n} + \frac{h_{j+1}}{6}\, q^{n*}$$

Hence $\left|b_j^n\right| - \left|a_j^n\right| - \left|c_j^n\right|$

$$\geqslant \frac{2(h_j+h_{j+1})\bar{p}_*^n}{3k_n} + \frac{h_j\bar{p}_*^n}{3k_n} + \frac{h_{j+1}\bar{p}_*^n}{3k_n}$$

$$- \frac{(h_j+h_{j+1})q^{n^*}}{3} - \frac{h_j}{6}q^{n^*} - \frac{h_{j+1}}{6}q^{n^*}$$

$$= (h_j+h_{j+1}) \left\{ \frac{\bar{p}_*^n}{k_n} - \frac{q^{n^*}}{2} \right\}$$

> 0 since by assumption $k_n < \dfrac{2\bar{p}_*^n}{q^{n^*}}$

Cor. 2.2

In the special case when $p \equiv 1$, $q \equiv 0$ in (1.1), i.e. for the inhomogeneous heat equation

$$y_t = y_{xx} - f(x,t)$$

subject to the initial and boundary condition (1.2) there is always a unique solution to the matrix equations (2.2).

Proof.

With $p = 1$, $q = 0$ the coefficients (2.3) become

$$(2.5) \qquad a_j^n = \frac{h_j}{3k} - \frac{1}{h_j}$$

$$b_j^n = \frac{2(h_j+h_{j+1})}{3k_n} + \frac{1}{h_j} + \frac{1}{h_{j+1}}$$

$$c_j^n = \frac{h_{j+1}}{3k_n} - \frac{1}{h_{j+1}}$$

$$d_0^n = g_0(t_n)$$

$$d_J^n = g_1(t_n)$$

$$d_j^n = \left(\frac{h_j}{3k_n} + \frac{1}{h_j}\right) U_{j-1}^{n-1} + \left(\frac{2(h_j+h_{j+1})}{3k_n} - \frac{1}{h_j} - \frac{1}{h_{j+1}}\right) U_j^{n-1}$$

$$+ \left(\frac{h_{j+1}}{3k_n} + \frac{1}{h_{j+1}}\right) U_{j+1}^{n-1}$$

$$+ \frac{1}{6}\left\{ h_j(f_{j-1}^n + f_{j-1}^{n-1}) + 2(h_j+h_{j+1})(f_j^n + f_j^{n-1}) + h_{j+1}(f_{j+1}^n + f_{j+1}^{n-1}) \right\}$$

$$(1 \leqslant j \leqslant J-1)$$

So $\quad |b_j^n| - |a_j^n| - |c_j^n|$

$$= \frac{2(h_j+h_{j+1})}{3k_n} + \frac{1}{h_j} + \frac{1}{h_{j+1}} - \left|\frac{h_j}{3k_n} - \frac{1}{h_j}\right| - \left|\frac{h_{j+1}}{3k_n} - \frac{1}{h_{j+1}}\right|$$

$$\geqslant \frac{2(h_j+h_{j+1})}{3k_n} + \frac{1}{h_j} + \frac{1}{h_{j+1}} - \frac{h_j}{3k_n} - \frac{1}{h_j} - \frac{h_{j+1}}{3k_n} - \frac{1}{h_{j+1}}$$

$$= \frac{h_j+h_{j-1}}{3k_n} > 0$$

I.3 Consistency of the Difference Scheme.

Theorem 3.1

The difference scheme (2.1) is consistent to second order accuracy with the problem (1.1, 1.2).

Proof.

Define the local truncation error τ_j^n by

$$\tau_j^n = L_h y_j^n$$

where y is the solution of the continuous problem (1.1, 1.2).

Taylor expand to derive the following:

$$(3.1)\qquad \frac{\bar{p}_j^n y_j^n - \bar{p}_j^{n-1} y_j^{n-1}}{k_n} = \frac{((\bar{p}y)_t)_j^n + ((\bar{p}y)_t)_j^{n-1}}{2} - \frac{k_n^2}{12}((\bar{p}y)_{ttt})_j^{n-\frac{1}{2}}$$

+ higher order terms.

$$(3.2)\quad \frac{\dfrac{y_{j+1}^{n}-y_{j}^{n}}{h_{j+1}} - \dfrac{y_{j}^{n}-y_{j-1}^{n}}{h_{j}}}{\frac{1}{2}(h_{j}+h_{j+1})}$$

$$= \frac{1}{3}\left\{\frac{h_{j}}{h_{j}+h_{j+1}}(y_{xx})_{j-1}^{n} + 2(y_{xx})_{j}^{n} + \frac{h_{j+1}}{h_{j}+h_{j+1}}(y_{xx})_{j+1}^{n}\right\}$$

$$-\frac{1}{12}\left(\frac{h_{j}^{3}+h_{j+1}^{3}}{h_{j}+h_{j+1}}\right)(y_{xxxx})_{j}^{n} \quad + \text{ higher order terms}$$

Using the identities (3.1) and (3.2) and the fact that y satisfies the differential equation (1.1) we see that:

$$(3.3)\quad \tau_{j}^{n} = \frac{1}{24}\left\{\frac{h_{j}^{3}+h_{j+1}^{3}}{h_{j}+h_{j+1}}\right\}\left\{(y_{xxxx})_{j}^{n} + (y_{xxxx})_{j}^{n-1}\right\}$$

$$-\frac{k_{n}^{2}}{36}\left\{\frac{h_{j}}{h_{j}+h_{j+1}}((py)_{ttt})_{j-1}^{n-\frac{1}{2}} + 2((py)_{ttt})_{j}^{n-\frac{1}{2}} + \frac{h_{j+1}}{h_{j}+h_{j+1}}((py)_{ttt})_{j+1}^{n-\frac{1}{2}}\right\}$$

$+$ higher order terms

If we let $h = \max_{0 \leq j \leq J} h_j$

and $k = \max_{1 \leq n \leq N} k_n$

then (3.3) shows that

$$\tau_j^n = O(h^2 + k^2)$$

I.4 Stability of the Difference Scheme.

In this section it will be shown that the difference scheme defined by (2.1) applied to the problem

$$(4.1) \qquad \begin{cases} py_t = y_{xx} + qy \\ y(x,0) = g(x) \\ y(0,t) = g_0(t) \\ y(1,t) = g_1(t) \end{cases}$$

is stable in the sense of Von Neumann.

We have to make the following assumptions:

(4.2) The net $R_h(T)$ is uniform.

(i.e. $h_j = h \quad (1 \leq j \leq J)$; $k_n = k \quad (1 \leq n \leq N)$)

(4.3) For each n $(0 \leq n \leq N)$ the approximate solution U_j^n $(0 \leq j \leq J)$ is periodic with period 1.

(4.4) The coefficient functions p and q are constant with $p > 0$ and $q < 0$.

The basic idea of a Von Neumann stability analysis is to write the finite difference solution as a Fourier series and then to show that none of the components can grow in amplitude as time increases.

Under the assumptions (4.2, 4.4) the difference equation for (4.1) is:

$$(4.5)\quad \left\{\frac{hp}{3k}-\frac{1}{h}-\frac{hq}{6}\right\}U_{j-1}^{n}+\left\{\frac{4hp}{3k}+\frac{2}{h}-\frac{2hq}{3}\right\}U_j^{n}+\left\{\frac{hp}{3k}-\frac{1}{h}-\frac{hq}{6}\right\}U_{j+1}^{n}$$

$$=\left\{\frac{hp}{3k}+\frac{1}{h}+\frac{hq}{6}\right\}U_{j-1}^{n-1}+\left\{\frac{4hp}{3k}-\frac{2}{h}+\frac{2hq}{3}\right\}U_j^{n-1}+\left\{\frac{hp}{3k}+\frac{1}{h}+\frac{hq}{6}\right\}U_{j+1}^{n}$$

By (4.3) we can write

$$(4.6)\quad \begin{cases} U^n(x)=\displaystyle\sum_{w=-\infty}^{\infty} c_w^n e^{iw2\pi x} \\ U^{n-1}(x)=\displaystyle\sum_{w=-\infty}^{\infty} c_w^{n-1} e^{iw2\pi x} \end{cases}$$

where $\left\{c_w^n\right\}$ and $\left\{c_w^{n-1}\right\}$ are the Fourier coefficients of $U^n(x)$ and $U^{n-1}(x)$ respectively.

Using (4.6) in (4.5) we deduce that the Fourier coefficients must satisfy the following relation:

$$(4.7)\quad \frac{c_w^n}{c_w^{n-1}} = \frac{\left(\frac{hp}{3k}+\frac{1}{h}+\frac{hq}{6}\right)e^{-i\xi}+\left(\frac{4hp}{3k}-\frac{2}{h}+\frac{2hq}{3}\right)+\left(\frac{hp}{3k}+\frac{1}{h}+\frac{hq}{6}\right)e^{i\xi}}{\left(\frac{hp}{3k}-\frac{1}{h}-\frac{hq}{6}\right)e^{-i\xi}+\left(\frac{4hp}{3k}+\frac{2}{h}-\frac{2hq}{3}\right)+\left(\frac{hp}{3k}-\frac{1}{h}-\frac{hq}{6}\right)e^{i\xi}}$$

where $\xi = 2\pi wh$

Using the fact that $e^{i\xi} + e^{-i\xi} = 2(1-2\sin^2\xi/2)$ we get

$$\frac{c_w^n}{c_w^{n-1}} = \frac{\left(\frac{4hp}{3k}-\frac{2}{h}+\frac{2hq}{3}\right)+2\left(\frac{hp}{3k}+\frac{1}{h}+\frac{hq}{6}\right)(1-2\sin^2\xi/2)}{\left(\frac{4hp}{3k}+\frac{2}{h}-\frac{2hq}{3}\right)+2\left(\frac{hp}{3k}-\frac{1}{h}-\frac{hq}{6}\right)(1-2\sin^2\xi/2)}$$

$$= \frac{\left(\frac{2hp}{k}-\frac{4hp}{3k}\sin^2\xi/2\right)-\left(4\left(\frac{1}{h}+\frac{hq}{6}\right)\sin^2\xi/2-hq\right)}{\left(\frac{2hp}{k}-\frac{4hp}{3k}\sin^2\xi/2\right)+\left(4\left(\frac{i}{h}+\frac{hq}{6}\right)\sin^2\xi/2-hq\right)}$$

Upon studying this last expression and recalling that

$p > 0$ and $q < 0$

we conclude that

$$\left|\frac{c_w^n}{c_w^{n-1}}\right| \leq 1$$

and hence stability has been established.

I.5 Equivalence of the Finite Difference Scheme and the Collocation Scheme.

The purpose of this section is to show that the collocation scheme defined by (1.3,1.4,1.5) is equivalent to the finite difference scheme (2.1).

Before establishing this fact in Theorem 5.3 we shall state a number of well known properties of cubic splines that are needed in the proof of Theorem 5.3.

Since we have already shown that the difference scheme has a unique solution provided the conditions (2.4) hold the equivalence of the two schemes will then imply that under the same conditions there is a unique solution to the collocation equations. This consequence is given in Corollary 5.4.

The finite difference scheme only gives approximate values of the solution at the mesh points. However, in Corollary 5.5 we shall show how approximations to first and second derivatives at the mesh points as well as approximations to the solution and itős first two derivatives at intermediate points can be obtained easily from the solution to the difference equations.

Lemma 5.1 Let U_j^n $(0 \leq j \leq J; \quad 1 \leq n \leq N)$ be the unique solution of the finite difference equations (2.1) subject to the conditions (2.4). Then for each n $(1 \leq n \leq N)$ there is a unique cubic spline S^n that interpolates the U_j^n of the mesh points k_j $(0 \leq j \leq J)$ and satisfies:

$$(S_{xx})_0^n = 2\left\{\frac{p_0^n S_0^n - p_0^{n-1} S_0^{n-1}}{k_n}\right\} - q_0^n S_0^n - f_0^n - (S_{xx})_0^{n-1} - q_0^{n-1} S_0^{n-1} - f_0^{n-1}$$

$$(S_{xx})_J^n = 2\left\{\frac{p_J^n S_J^n - p_J^{n-1} S_J^{n-1}}{k_n}\right\} - q_J^n S_J^n - f_J^n - (S_{xx})_J^{n-1} - q_J^{n-1} S_J^{n-1} - f_J^{n-1}$$

where $(S_{xx})_0^0 = g_{xx}(0)$, $(S_{xx})_J^0 = g_{xx}(1)$,

$S_0^0 = g(0)$ and $S_J^0 = g(1)$.

Proof.

Clearly the assertion follows if we can show that for arbitrary data-points $\left\{(x_j, y_j)\right\}_{j=0}^{J}$ with

$$0 = x_0 < x_1 < \ldots . < x_J = 1$$

and for arbitrary numbers α and β there exists a unique cubic spline S such that

$$S(x_j) = y_j \qquad (0 \leq j \leq J)$$

$$S_{xx}(x_0) = \alpha$$

$$S_{xx}(x_J) = \beta$$

But this is a standard interpolation result, that can easily be shown by making use of relation (5.1) of the following Lemma.

Lemma 5.2 Let S be a cubic spline in the interval $[0,1]$ with knots $0 = x_0 < x_1 < \ldots < x_J = 1$

Then S satisfies

$$(5.1) \quad \frac{1}{3}\left\{ \frac{h_j}{h_j+h_{j+1}}(S_{xx})_{j-1} + 2(S_{xx})_j + \frac{h_{j+1}}{h_j+h_{j+1}}(S_{xx})_{j+1} \right\} = \frac{\dfrac{S_{j+1}-S_j}{h_{j+1}} - \dfrac{S_j - S_{j-1}}{h_j}}{\frac{1}{2}(h_j+h_{j+1})} \qquad (1 \leq j \leq J-1)$$

(5.2)
$$(S_x)_j = \frac{S_j - S_{j-1}}{h_j} + \frac{h_j}{6}\left\{2(S_{xx})_j + (S_{xx})_{j-1}\right\} \quad (1 \leq j \leq J)$$

(5.3)
$$(S_x)_j = \frac{S_{j+1} - S_j}{h_{j+1}} - \frac{h_{j+1}}{6}\left\{2(S_{xx})_j + (S_{xx})_{j+1}\right\} \quad (0 \leq j \leq J-1)$$

Proof.

These identities are easy to obtain, e.g. by using Taylor expansions for S noting that

$$\frac{d^k}{dx^k} S = 0 \quad \text{for} \quad k \geq 4$$

See for example [9 pp. 31-32] .

Theorem 5.3

Let $\left\{ U_j^n \right\}$ $(0 \leq j \leq J \quad 1 \leq n \leq N)$ be the unique solution of the difference equations (2.1) subject to the conditions (2.4).

(5.4) For each n $(1 \leq n \leq N)$ let S^n be the unique cubic spline interpolant of $\left\{ U_j^n \right\}$ $(0 \leq j \leq J,\ \ 1 \leq n \leq N)$ satisfying

$$(S_{xx})_0^n = 2\left\{\frac{p_0^n S_0^n - p_0^{n-1} S_0^{n-1}}{k_n}\right\} - q_0^n S_0^n - f_0^n - (S_{xx})_0^{n-1} - q_0^{n-1} S_0^{n-1} - f_0^{n-1}$$

$$(S_{xx})_J^n = 2\left\{\frac{p_J^n S_J^n - p_J^{n-1} S_J^{n-1}}{k_n}\right\} - q_J^n S_J^n - f_J^n - (S_{xx})_J^{n-1} - q_J^{n-1} S_J^{n-1} - f_J^{n-1}$$

(5.5) Let S^0 be the unique cubic spline interpolant of the initial data $g(x)$ at the points $\left\{ x_j \right\}$ $(0 \leq j \leq J)$ satisfying

$$(S_{xx})_0^0 = g_{xx}(0)$$

$$(S_{xx})_J^0 = g_{xx}(1)$$

Then for each n $(1 \leq n \leq N)$, S^n satisfies the collocation equations (1.3, 1.4, 1.5). Conversely assume that S^n is a solution of the collocation equations (1.3, 1.4, 1.5). Then for each n $(1 \leq n \leq N)$, S^n satisfies the difference equations (2.1).

Proof.

Let $\{S^n\}$ $(0\le n\le N)$ be the cubic splines as defined in 5.4 and 5.5. (These are uniquely determined by Lemma 5.1). Then S^n satisfies the difference equations (2.1) for $(1\le n\le N)$. Also S^n satisfies the relation (5.1) for $(0\le n\le N)$. Hence for $(1\le n\le N)$ we have that

$$\frac{1}{3}\left\{\frac{h_j}{h_j+h_{j+1}}\left(\frac{p^n_{j-1}S^n_{j-1}-p^{n-1}_{j-1}S^{n-1}_{j-1}}{k_n}\right)+2\left(\frac{p^n_jS^n_j-p^{n-1}_jS^{n-1}_j}{k_n}\right)\right.$$
$$\left.+\frac{h_{j+1}}{h_j+h_{j+1}}\left(\frac{p^n_{j+1}S^n_{j+1}-p^{n-1}_{j+1}S^{n-1}_{j+1}}{k_n}\right)\right\}$$

$$(5.6)\quad -\frac{1}{6}\left\{\frac{h_j}{h_j+h_{j+1}}(S_{xx})^n_{j-1}+2(S_{xx})^n_j+\frac{h_{j+1}}{h_j+h_{j+1}}(S_{xx})^n_{j+1}\right.$$
$$\left.+\frac{h_j}{h_j+h_{j+1}}(S_{xx})^{n-1}_{j-1}+2(S_{xx})^{n-1}_j+\frac{h_{j+1}}{h_j+h_{j+1}}(S_{xx})^{n-1}_{j+1}\right\}$$

$$-\frac{1}{6}\left\{\frac{h_j}{h_j+h_{j+1}}(q^n_{j-1}S^n_{j-1}+q^{n-1}_{j-1}S^{n-1}_{j-1})+2(q^n_jS^n_j+q^{n-1}_jS^{n-1}_j)\right.$$
$$\left.+\frac{h_{j+1}}{h_j+h_{j+1}}(q^n_{j+1}S^n_{j+1}+q^{n-1}_{j+1}S^{n-1}_{j+1})\right\}$$

$$-\frac{1}{6}\left\{\frac{h_j}{h_j+h_{j+1}}(f^n_{j-1}+f^{n-1}_{j-1})+2(f^n_j+f^{n-1}_j)+\frac{h_{j+1}}{h_j+h_{j+1}}(f^n_{j+1}+f^{n-1}_{j+1})\right\}\equiv 0 \quad 1\le j\le J-1$$

Let

$$\widetilde{L}\, s_j^n = \frac{p_j^n s_j^n - p_j^{n-1} s_j^{n-1}}{k_n} - \frac{1}{2}\left\{ (s_{xx})_j^n + q_j^n s_j^n + f_j^n + (s_{xx})_j^{n-1} + q_j^{n-1} s_j^{n-1} + f_j^{n-1} \right\}$$

Then (5.6) becomes

$$(5.7)\quad \frac{h_j}{h_j+h_{j+1}}\, \widetilde{L}\, s_{j-1}^n + 2\,\widetilde{L}\, s_j^n + \frac{h_{j+1}}{h_j+h_{j+1}}\, \widetilde{L}\, s_{j+1}^n = 0$$

$$(1 \leq j \leq J-1\ ,\ 1 \leq n \leq N).$$

and by hypothesis 5.4 we have that

$$\widetilde{L}\, s_0^n = \widetilde{L}\, s_J^n = 0 \qquad (1 \leq n \leq N).$$

We can consider (5.7) as a system of linear equations in the unknown $\left\{ \widetilde{L}\, s_j^n \right\}_{j=0}^{J}$ for each $(1 \leq n \leq N)$ with the right-hand side being the zero vector.

Since

$$\frac{h_j}{h_j+h_{j+1}} + \frac{h_{j+1}}{h_j+h_{j+1}} = 1 < 2$$

we must have that

$$\widetilde{L}\, s_j^n = 0 \quad (0 \leq j \leq J\ ,\ 1 \leq n \leq N)$$

But this implies that for each n ($1 \leqslant n \leqslant N$) S^n satisfies the collocation equation (1.5). Clearly for each n ($1 \leqslant n \leqslant N$) S^n also satisfies the boundary conditions (1.4) and hence the first assertion has been proved. Conversely if we assume that for each n ($1 \leqslant n \leqslant N$) S^n is a solution of the collocation equations (1.3, 1.4, 1.5) then

$$\tilde{L} S_j^n = 0 \quad (0 \leqslant j \leqslant J, \quad 1 \leqslant n \leqslant N)$$

Therefore

$$\frac{1}{3}\left\{ \frac{h_j}{h_j+h_{j+1}} \tilde{L} S_{j-1}^n + 2\tilde{L} S_j^n + \frac{h_{j+1}}{h_j+h_{j+1}} S_{j+1}^n \right\} = 0 \qquad (1 \leqslant j \leqslant J-1 \ , \ 1 \leqslant n \leqslant N)$$

This relation, however, is identical to (5.6) and using (5.1) it follows that each S^n satisfies the difference equation (2.1). As an immediate consequence of Theorem 5.3 we have the following:

Cor. 5.4 Under the conditions (2.4) of Theorem 2.1 there is a unique solution S^n $(1 \leqslant n \leqslant N)$ to the collocation equations (1.3, 1.4, 1.5) with

$$S_j^n = U_j^n \qquad (0 \leqslant j \leqslant J; \;\; 1 \leqslant n \leqslant N)$$

where

U_j^n $(0 \leqslant j \leqslant J; \;\; 1 \leqslant n \leqslant N)$ is the unique solution of the difference equations (2.1).

Cor. 5.5 Given the solution U_j^n $(0 \leqslant j \leqslant J; \;\; 1 \leqslant n \leqslant N)$ of the finite difference equations (2.1) and setting

$$S_j^n = U_j^n \qquad (0 \leqslant j \leqslant J; \;\; 1 \leqslant n \leqslant N)$$

we can explicitly compute

$(S_{xx})_j^n$ and $(S_x)_j^n$ $(0 \leqslant j \leqslant J; \;\; 1 \leqslant n \leqslant N)$ by

$$(5.8)\quad (S_{xx})_j^n = 2\left\{\frac{p_j^n S_j^n - p_j^{n-1} S_j^{n-1}}{k_n}\right\} = q_j^n S_j^n - f_j^n - (S_{xx})_j^{n-1} - q_j^{n-1} S_j^{n-1} - f_j^{n-1}$$

$$(0 \leqslant j \leqslant J; \quad 1 \leqslant n \leqslant N)$$

$$(5.9)\quad (S_x)_j^n = \frac{S_{j+1}^n - S_j^n}{h_{j+1}} - \frac{h_{j+1}}{6}\left\{2(S_{xx})_j^n + (S_{xx})_{j+1}^n\right\}$$

$$(0 \leqslant j \leqslant J-1; \quad 1 \leqslant n \leqslant N)$$

$$(5.10)\quad (S_x)_J^n = \frac{S_J^n - S_{J-1}^n}{h_J} + \frac{h_J}{6}\left\{2(S_{xx})_J^n + (S_{xx})_{J-1}^n\right\}$$

where S^0 is again taken to be the cubic spline interpolant of the initial data $g(x)$ at the points $\{x_j\}_{j=0}^{J}$ satisfying:

$$(S_{xx})_0^0 = g_{xx}(0)$$

and

$$(S_{xx})_J^0 = g_{xx}(1)$$

Moreover if $x_j < x < x_{j-1}$ then

$$(5.11)\quad (S_{xx})^n(x) = \frac{x_{j+1}-x}{h_{j+1}}(S_{xx})_j^n + \frac{x-x_j}{h_{j+1}}(S_{xx})_{j+1}^n$$

$$(5.12)\quad (S_x)^n(x) = (S_x)_j^n + (x-x_j)(S_{xx})_j^n + \frac{(x-x_j)^2}{2}\left\{\frac{(S_{xx})_{j+1}^n-(S_{xx})_j^n}{h_{j+1}}\right\}$$

$$(5.13)\quad S^n(x) = \frac{(x_{j+1}-x)S_j^n+(x-x_j)S_{j+1}^n}{h_{j+1}}$$

$$- \frac{(x_{j+1}-x)(x-x_j)}{6}\left\{(S_{xx})^n(x) + (S_{xx})_j^n + (S_{xx})_{j+1}^n\right\}$$

Proof.

(5.8) follow from the collocation condition (1.5),

(5.9) and (5.10) follow from Lemma (5.2), and (5.11),

(5.12) and (5.13) are simple interpolation formulas.

For example (5.11) represents linear interpolation, since the second derivative of a cubic spline is a continuous piece wise linear function.

I.6 The Algorithm for Solving the Collocation Equations.

The algorithm for solving the problem (1.1) subject to the initial and boundary conditions (1.2) is in fact implied by Cor. 5.4 and Cor. 5.5. Below it will be stated more precisely, using the standard L _ U decomposition for tridiagonal matrices [10 pp. 55 - 56] to solve the linear equation (2.2)

Given a net on $R(T) = [0,1] \times [0,T]$ with $x_0 = 0$ $x_J = 1$ $t_0 = 0$ $t_N = T$ and netspacings

$$h_j = x_j - x_{j-1} \qquad (1 \leq j \leq J)$$

$$k_n = t_n - t_{n-1} \qquad (1 \leq n \leq N)$$

the algorithm will give approximations

$$\left.\begin{aligned} U_j^n &\equiv S_j^n && \text{to } y_j^n \\ V_j^n &\equiv (S_x)_j^n && \text{to } (y_x)_j^n \\ W_j^n &\equiv (S_{xx})_j^n && \text{to } (y_{xx})_j^n \end{aligned}\right\} \qquad (0 \leq j \leq J; \quad 1 \leq n \leq N)$$

First we have to compute the cubic spline interpolant S^0 of the initial data $g(x)$ at the points $\left\{x_j\right\}_{j=0}^{J}$ satisfying the endpoint conditions

$$(S_{xx})_0^0 = g_{xx}(0)$$

and

$$(S_{xx})_J^0 = g_{xx}(1)$$

However, since we only need $(S_{xx})_j^0$ $(0 \leq j \leq J)$ for subsequent computations, these values can be computed easily by making use of relation (5.1) of Lemma 5.2. This relation leads to a matrix equation of the form:

$$
(6.1) \qquad
\begin{vmatrix}
b_1^0 & c_1^0 & & \\
a_2^0 & b_2^0 & c_2^0 & \\
 & \ddots & \ddots & \ddots \\
 & & a_{J-1}^0 & b_{J-1}^0
\end{vmatrix}
\cdot
\begin{vmatrix}
(S_{xx})_1^0 \\
(S_{xx})_2^0 \\
\vdots \\
(S_{xx})_{J-1}^0
\end{vmatrix}
=
\begin{vmatrix}
d_1^0 \\
d_1^0 \\
\vdots \\
d_{J-1}^0
\end{vmatrix}
$$

with

$$a_j^0 = \frac{h_j}{h_j + h_{j+1}} \qquad (2 \leq j \leq J-1)$$

$$b_j^0 = 2 \qquad (1 \leq j \leq J-1)$$

$$c_j^0 = \frac{h_{j+1}}{h_j + h_{j+1}} \qquad (1 \leq j \leq J-2)$$

and

$$d_1^0 = 6\left\{\frac{\dfrac{g(x_2)-g(x_1)}{h_2} - \dfrac{g(x_1)-g(x_0)}{h_1}}{(h_1 + h_2)}\right\} - g_{xx}(x_0)\left(\frac{h_1}{h_1+h_2}\right)$$

$$d_j^0 = 6\left\{\frac{\dfrac{g(x_{j+1})-g(x_j)}{h_{j+1}} - \dfrac{g(x_j)-g(x_{j-1})}{h_j}}{(h_j + h_{j+1})}\right\} \quad (2 \leq j \leq J-2)$$

$$d_{J-1}^n = 6\left\{\frac{\dfrac{g(x_J)-g(x_{J-1})}{h_J} - \dfrac{g(x_{J-1})-g(x_{J-2})}{h_{J-1}}}{(h_{J-1} + h_J)}\right\} - g_{xx}(x_J)\left(\frac{h_J}{h_{J-1}+h_J}\right)$$

Applying the L_U decomposition algorithm for tridiagonal matrices, with intermediate quantities α_j^0, γ_j^0 and w_j^0, we can now solve the system (6.1) by:

$$\alpha_1^0 = b_1^0$$

$$\gamma_1^0 = c_1^0 \Big/ \alpha_1^0$$

$$\alpha_j^0 = b_j^0 - a_j^0 \, \gamma_{j-1}^0 \qquad (2 \leq j \leq J-1)$$

$$\gamma_j^0 = c_j^0 \Big/ \alpha_j^0 \qquad (2 \leq j \leq J-2)$$

$$w_1^0 = d_1^0$$

$$w_j^0 = (d_j^0 - a_j^0 w_{j-1}^0) \Big/ \alpha_j^0 \qquad (2 \leq j \leq J-1)$$

$$(S_{xx})_J^0 = g_{xx}(x_J) = g_{xx}(1)$$

$$(S_{xx})_{J-1}^0 = w_{J-1}^0$$

$$(S_{xx})_j^0 = w_j^0 - \gamma_j^0 (S_{xx})_{j+1}^0 \qquad (J-2 \geq j \geq 1)$$

$$(S_{xx})_0^0 = g_{xx}(x_0) = g_{xx}(0)$$

We now initialize U_j^0 and W_j^0 by

$$\left.\begin{aligned} U_j^0 &= g(x_j) \\ W_j^0 &= (S_{xx})_j^0 \end{aligned}\right\} \quad (0 \leq j \leq J)$$

<u>Let n = 1</u>

(*) Next compute the coefficients a_j^n, b_j^n, c_j^n and d_j^n of the matrix equation (2.2) as defined by (2.3), or by (2.5) in case of the inhomogeneous heat equation. Again to solve (2.2) we use the $\underline{L}\,U$ decomposition algorithm, with intermediate quantities α_j^n, γ_j^n and w_j^n, which leads to the following computations:

$$\alpha_1^n = b_1^n$$

$$\gamma_1^n = c_1^n / \alpha_1^n$$

$$\alpha_j^n = b_j^n - a_j^n \gamma_{j-1}^n \qquad (2 \leq j \leq J-1)$$

$$\gamma_j^n = c_j^n / \alpha_j^n \qquad (2 \leq j \leq J-2)$$

$$w_1^n = d_1^n - a_1^n g_0(t_n)$$

$$w_j^n = (d_j^n - a_j^n w_{j-1}^n) / \alpha_j^n \qquad (2 \leq j \leq J-2)$$

$$w_{J-1}^n = (d_{J-1}^n - c_{J-1}^n g_1(t_n) - a_{J-1}^n w_{J-2}^n) / \alpha_{J-1}$$

The approximations to the solution and its first two derivatives are now obtained as follows:

$$U_J^n = g_1(t_n)$$

$$U_{J-1}^n = w_{J-1}^n$$

$$U_j^n = w_j^n - \gamma_j^n U_{j+1}^n \qquad (J-2 \geq j \geq 1)$$

$$U_0^n = g_0(t_n)$$

$$W_j^n = 2\left\{\frac{p_j^n U_j^n - p_j^{n-1} U_j^{n-1}}{k_n}\right\} - q_j^n U_j^n - f_j^n - W_j^{n-1} - q_j^{n-1} U_j^{n-1} - f_j^{n-1}$$

$$(0 \leq j \leq J)$$

$$V_j^n = \frac{U_{j+1}^n - U_j^n}{h_{j+1}} - \frac{h_{j+1}}{6}\left\{2W_j^n + W_{j+1}^n\right\} \qquad (0 \leq j \leq J-1$$

$$V_J^n = \frac{U_J^n - U_{J-1}^n}{h_J} + \frac{h_J}{6}\left\{2W_J^n + W_{J-1}^n\right\}$$

Starting at (*) we repeat the same computations with n increasing from 2 to M.

PART II. Results of Numerical Computations.

The collocation scheme was used to obtain approximate solutions to four differential equations. For each problem solutions were computed with various mesh sizes. The results are given below, as well as those obtained by applying Keller's Box Scheme [11] and the Crank-Nicolson scheme [6] to these problems.

In these tables J denotes the number of mesh-intervals, both in the x-direction and in the t-direction. Each problem was solved on the unit square, so that for a uniform mesh the mesh-spacings in the x- and t- directions are given by $1/J$. A non-uniform mesh was used in Problem 4 only. Further by e, e_x and e_{xx} we denote the maximum error in the approximate solution and in the approximate first and second derivatives respectively, the maximum being taken over the mesh points. The quantity between brackets is the observed rate of convergence, obtained by computing the value of

$$\frac{\log\left(\dfrac{e_i}{e_{i-1}}\right)}{\log\left(\dfrac{J_{i-1}}{J_i}\right)}$$

Problem 1.

The first problem was to solve the following homogeneous heat equation:

$$y_t = y_{xx} \qquad (0 \le x \le 1; \quad 0 \le t \le 1)$$

$$y(x,0) = e^x$$

$$y(0,t) = e^t$$

$$y(1,t) = e^{t+1}$$

which has $y(x,t) = e^{x+t}$ as its unique solution. The mesh was taken to be uniform, i.e. $h = k = 1/J$. The results are given in Table 1. We note that solution of the collocation scheme converges at the rate of 4.0 to the solution $y(x,t)$ of the continuous problem at the mesh points. Such an accuracy cannot be expected in general, however, The reason that it happens here is that apparently for this particular problem the next two terms of the error expansion (3.4) cancel. Further we note that the error e for the Box-scheme is approximately one half of the error e for the Crank-Nicolson scheme.

Problem 2.

The second problem was to solve the following inhomogeneous heat equation:

$$y_t = y_{xx} + \cos(x+t) - \sin(x+t) \qquad (0 \leq x \leq 1;\ 0 \leq t \leq 1)$$

$$y(x,0) = \sin(x)$$

$$y(0,t) = \sin(t)$$

$$y(1,t) = \sin(t+1)$$

which has $y(x,t) = \sin(x+t)$ as its unique solution. As in Problem 1, this solution is particularly smooth and well-behaved so that good results may be expected. The mesh was taken to be uniform. The results are given in Table 2, and indicate that the cubic spline collocation scheme is second order accurate in its approximation to the solution as well as in its approximation to the first and second derivative of the solution. In this problem the Crank-Nicolson scheme gives the best approximation to the solution.

TABLE 1

	Cubic Spline Scheme			Box Scheme		C. N.
J	e	e_x	e_{xx}	e	e_x	e
5	$.456^{-5}$	$.564^{-3}$	$.255^{-1}$	$.173^{-2}$	$.162^{-1}$	$.340^{-2}$
10	$.287^{-6}$ (4.00)	$.677^{-4}$ (3.06)	$.783^{-2}$ (1.70)	$.432^{-3}$ (2.00)	$.404^{-2}$ (2.00)	$.861^{-3}$ (1.98)
20	$.181^{-7}$ (4.00)	$.833^{-5}$ (3.02)	$.203^{-2}$ (1.95)	$.109^{-3}$ (2.00)	$.101^{-2}$ (2.00)	$.217^{-3}$ (2.00)
40	$.113^{-8}$ (4.00)	$.103^{-5}$ (3.02)	$.517^{-3}$ (1.97)	$.272^{-4}$ (2.00)	$.253^{-3}$ (2.00)	$.543^{-4}$ (2.00)

TABLE 2

	Cubic Spline Scheme			Box Scheme		C. N.
JJ	e	e_x	e_{xx}	e	e_x	e
5	$.561^{-3}$	$.257^{-2}$	$.663^{-2}$	$.970^{-3}$	$.777^{-2}$	$.330^{-3}$
10	$.142^{-3}$ (1.98)	$.614^{-3}$ (2.07)	$.166^{-2}$ (2.00)	$.213^{-3}$ (2.19)	$.177^{-2}$ (2.13)	$.826^{-4}$ (2.00)
20	$.355^{-4}$ (2.00)	$.148^{-3}$ (2.05)	$.417^{-3}$ (2.00)	$.529^{-4}$ (2.01)	$.428^{-3}$ (2.05)	$.208^{-4}$ (2.00)

Problem 3.

The third problem was to solve

$$y_t = y_{xx} + \frac{400(x-t+1)}{(1+200(x-t)^2)^2} - \frac{2(400(x-t))^2}{(1+200(x-t)^2)^3}$$

$$(0 \leq x \leq 1; \quad 0 \leq t \leq 1)$$

$$y(x,0) = \frac{1}{1+200x^2}$$

$$y(0,t) = \frac{1}{1+200t^2}$$

$$y(1,t) = \frac{1}{1+200(1-t)^2}$$

which has

$$y(x,t) = \frac{1}{1+200(x-t)^2}$$ as its unique solution.

The solution of this problem involves a narrow wave travelling along the line $t = x$. The mesh was again taken to be uniform, since what may be a good choice of mesh points in the x-direction at one time-level, will be a poor choice at the next time-level. The numerical results are given in Table 3. For this problem the cubic spline collocation scheme can be seen to give the best approximation to the solution and its first derivative.

The Box scheme shows a large error in the approximation to the first derivative, when J is small. In fact heavy oscillation was observed in the approximation to the first derivative of the solution, even where this derivative should be small. It has been noted in [7 pp.25-26] that the Box scheme does lead to such oscillations in certain problems with boundary conditions as above.

The rate of convergence does not approach 2.0 as clearly as in the preceding problem, however, this is usually the case when less well-behaved functions are used to test a scheme.

TABLE 3

	Cubic Spline Scheme			Box Scheme		C. N.
J	e	e_x	e_{xx}	e	e_x	e
10	$.464^{+1}$	$.249^{+2}$	$.632^{+2}$	$.533^{+1}$	$.648^{+2}$	$.524^{+1}$
20	$.220^{00}$ (4.40)	$.138^{+1}$ (4.17)	$.147^{+2}$ (2.10)	$.352^{00}$ (3.92)	$.230^{+2}$ (1.49)	$.344^{00}$ (3.93)
40	$.264^{-1}$ (3.06)	$.903^{00}$ (0.61)	$.232^{+2}$ (-0.66)	$.439^{-1}$ (3.00)	$.350^{+1}$ (2.72)	$.325^{-1}$ (3.40)
80	$.617^{-2}$ (2.10)	$.220^{00}$ (2.04)	$.109^{+2}$ (1.09)	$.922^{-2}$ (2.25)	$.502^{00}$ (2.80)	$.654^{-2}$ (2.31)

Problem 4.

Finally we consider the following differential equation:

$$y_t = y_{xx} - \frac{2tx^{20}}{(1+t^2)^2} - \frac{380x^{18}}{1+t^2} \qquad (0 \leq x \leq 1; \quad 0 \leq t \leq 1)$$

$$y(x,0) = x^{20}$$

$$y(0,t) = 0$$

$$y(1,t) = \frac{1}{1+t^2}$$

which has solution

$$y(x,t) = \frac{x^{20}}{1+t^2}$$

Since the solution involves a boundary layer near $x = 1$ it is reasonable to place more net points near $x = 1$ than else where.

Table 4 shows the results that were obtained with a uniform mesh, and Table 5 gives the results obtained with non-uniform mesh in the x-direction. The net spacings in the time direction were taken to be uniform in both cases. In the case of non-uniform netspacing in the x-direction with $J = 7$ the net points were:

$x_0 = 0.0$

$x_1 = 0.47$

$x_2 = 0.67$

$x_3 = 0.78$

$x_4 = 0.85$

$x_5 = 0.91$

$x_6 = 0.96$

$x_7 = 1.00$

With $J = 12$ the netpoints were chosen to be:

$x_0 = 0.0$	$x_7 = 0.87$
$x_1 = 0.47$	$x_8 = 0.90$
$x_2 = 0.61$	$x_9 = 0.934$
$x_3 = 0.69$	$x_{10} = 0.958$
$x_4 = 0.75$	$x_{11} = 0.980$
$x_5 = 0.80$	$x_{12} = 1.00$
$x_6 = 0.84$	

With J = 28, 43 the net points were chosen in a similar fashion.

For this problem the Box scheme gave the best results, and comparing Table 4 and Table 5 we note that considerable improvement in accuracy is obtained if we place more net points in the region where the solution changes most rapidly.

TABLE 4 (Uniform mesh)

	Cubic Spline Scheme			Box Scheme		C. N.
J	e	e_x	e_{xx}	e	e_x	e
7	$.892^{00}$	$.125^{+2}$	$.423^{+2}$	$.269^{00}$	$.908^{-1}$	$.514^{00}$
12	$.237^{00}$ (2.46)	$.476^{+1}$ (1.79)	$.267^{+2}$ (0.85)	$.995^{-1}$ (1.85)	$.357^{-1}$ (1.73)	$.192^{00}$ (1.83)
28	$.316^{+1}$ (2.38)	$.900^{00}$ (1.97)	$.875^{+1}$ (1.32)	$.154^{-1}$ (2.20)	$.705^{00}$ (1.91)	$.302^{-1}$ (2.18)
43	$.128^{-1}$ (2.11)	$.370^{00}$ (2.07)	$.437^{+1}$ (1.62)	$.630^{-2}$ (2.08)	$.302^{00}$ (1.98)	$.126^{-1}$ (2.04)

TABLE 5 (Non-uniform mesh)

	Cubic Spline Scheme			Box Scheme	
J	e	e_x	e_{xx}	e	e_x
7	$.109^{00}$	$.185^{+1}$	$.119^{+2}$	$.221^{-1}$	$.103^{+1}$
12	$.258^{-1}$ (2.66)	$.490^{00}$ (2.46)	$.377^{+1}$ (2.13)	$.478^{-2}$ (2.84)	$.269^{00}$ (2.49)
28	$.406^{-2}$ (2.18)	$.738^{-1}$ (2.24)	$.756^{00}$ (1.90)	$.517^{-3}$ (2.62)	$.438^{-1}$ (2.14)
43	$.163^{-2}$ (2.13)	$.271^{-1}$ (2.33)	$.330^{00}$ (1.93)	$.168^{-3}$ (2.62)	$.171^{-1}$ (2.19)

PART III. Application to the Stefan Problem.

III.1 Introduction.

In this section we shall indicate how our collocation method with cubic splines may be used to obtain an approximate solution to a moving boundary value problem, usually known as the Stefan problem.

The Stefan problem arises in certain physical processes that are governed by a parabolic partial differential equation, together with a moving boundary condition. As an example we mention the melting of ice.

We shall consider a simple type of moving boundary problem, namely that of finding $s(t)$ (the moving boundary) and $y(x,t)$ for which

$$
(1.1)\quad
\begin{aligned}
&\text{A)}\ \ y_t = y_{xx} + f(x,t) \qquad (0 \le x \le s(t),\ 0 \le t \le T) \begin{cases} s(0) = 1 \\ s(T) \geq 0 \end{cases} \\
&\text{B)}\ \ y(x,0) = g(x) \\
&\text{C)}\ \ y_x(0,t) = 0 \\
&\text{D)}\ \ y(s(t),t) = 0 \\
&\text{E)}\ \ \alpha^2 y_x(s(t),t) - \dot{s}(t) = H(t) \qquad \dot{s}(t) \equiv \frac{ds}{dt}
\end{aligned}
$$

(Condition (1.1 E) is the moving boundary condition).

We require s(t) to be strictly decreasing and $|\dot{s}(t)| < \infty$ for $(0 \leq t \leq T)$. For a discussion on the existence and uniqueness of solution to (1.1) see Friedman [8] or Cannon and Hill [2].

Numerical solution of the Stefan problem has been treated by for example J. Douglas, Jr. and T. M. Gallie, Jr. [4], who made use of an implicit (forward) finite difference scheme. Their analysis required the flux at the fixed boundary to be constant. Also we mention G. H. Meyer [12], who considered a more general moving boundary problem. By discretizing the time-variable he reduced the Stefan problem to a sequence of free boundary value problems of ordinary differential equations, which are solved by conversion to initial value problems.

III.2 Description of the Scheme.

First we shall replace the moving boundary condition (1.1.E) by an equivalent condition that does not involve the derivative $\dot{s}$ of the moving boundary. Since the derivative dy/dt is zero in the direction of the boundary s(t) it follows that

$$(2.1) \quad \dot{s}(t)y_x(s(t),t) = -y_t(s(t),t) = -y_{xx}(s(t),t)-f(s(t),t)$$

Using (2.1) the moving boundary condition (1.1.E) can now be written as

$$(2.2)\left\{H(t)-\alpha^2 y_x(s(t),t)\right\} y_x(s(t),t) = y_{xx}(s(t),t)+f(s(t),t)$$

The moving boundary condition written in form (2.2) will be used in later discussion.

Let a partition $0 = x_0 < x_1 < \ldots\ldots < x_J = 1$ of the unit interval $[0,1]$ be given. The time levels denoted by $0 = t_0 < t_1 < \ldots\ldots < t_n$ with $N \leq J-2$ are varying. Mesh spacings are given by

$$h_j = x_j - x_{j-1} \qquad (1 \leq j \leq J)$$

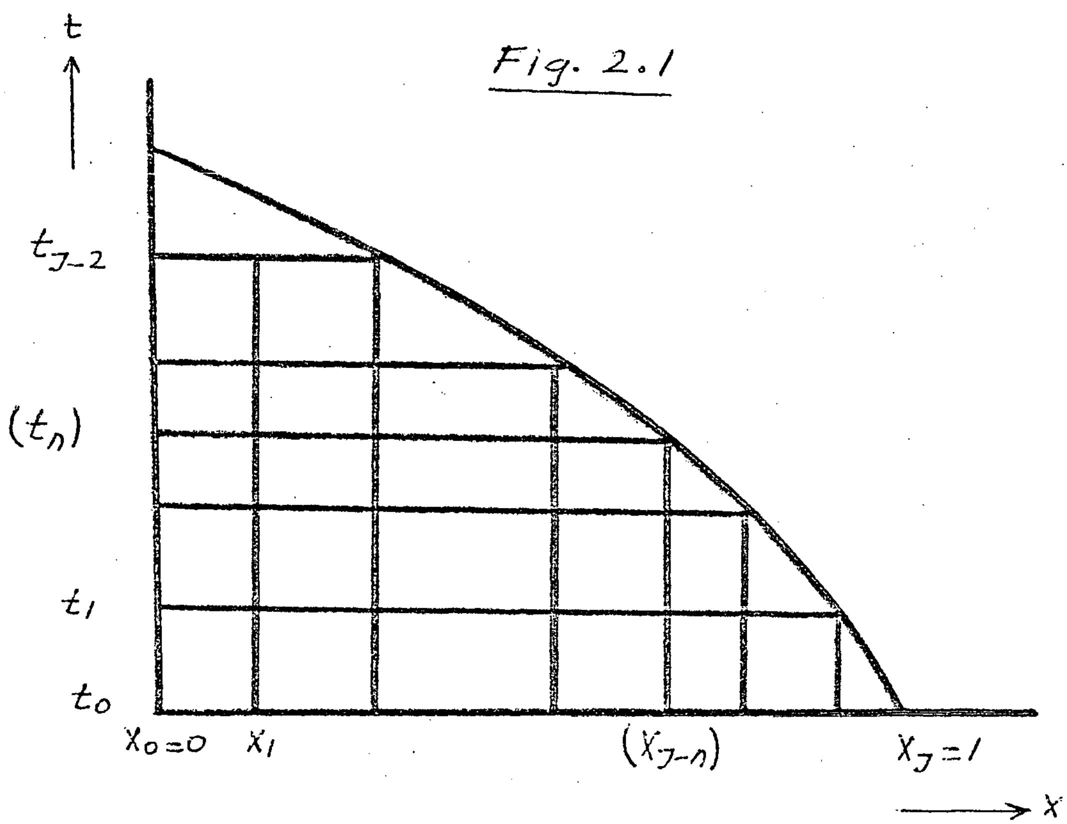
and

$$k_n = t_n - t_{n-1} \qquad (1 \leq n \leq N \leq J-2)$$

At time-level t_n the meshpoints are $\left\{ x_j \right\}_{j=0}^{J-n}$,

so that when proceeding from one time-level to the next one, the rightmost meshpoint will be dropped. At time-level t_n this rightmost meshpoint x_{J-n} is to be the approximation to the moving boundary. (See fig. 2.1).

Fig. 2.1



As in Part I we require the approximation to the solution $y(x,t)$ of (1.1) at each time t_n to be a cubic spline $S^n(x)$ satisfying:

The boundary conditions:

(2.3.A) $(S_x)^n_0 = 0$

(2.3.B) $S^n_{J-n} = 0$

and the collocation conditions:

(2.3.C) $$\frac{S^n_j - S^{n-1}_j}{k_n} = \frac{1}{2}\left\{(S_{xx})^n_j + (S_{xx})^{n-1}_j\right\} + \frac{1}{2}\left\{f^n_j + f^{n-1}_j\right\} \quad (0 \leq j \leq J-n)$$

The timesteps $\left\{k_n\right\}_{n=1}^{J-2}$ are unknown before hand; they will be determined by requiring that $S^n(x)$ satisfy the moving boundary condition (2.2). That is $S^n(x)$ must satisfy

(2.4) $$\left\{H(t_n) - \alpha^2 (S_x)^n_{J-n}\right\} (S_x)^n_{J-n} - (S_{xx})^n_{J-n} - f^n_{J-n} \equiv G(k_n, S^n) = 0$$

By the results of Part I we can, for given $S^{n-1}(x)$ and k_n, easily obtain a solution to the collocation scheme (2.3) by solving and equivalent finite difference scheme. This finite difference scheme again leads to matrix equations that involve only tridiagonal matrices, and that are therefore readily solved by the standard L_U decomposition algorithm[10, pp. 35 - 42] .

Approximations to the first two derivatives of the solution $y(x,t)$ can be obtained by explicit computation from the solution of the finite difference equations. These approximations are needed to compute the value of $G(k_n, S^n)$ as defined by (2.4). The basic idea of the scheme is to find k_n for which the solution $S^n(x)$ of the collocation equations (2.3) satisfies (2.4). The only place where non-linearity enters the scheme is in relation (2.4).

In Part I we did not consider boundary conditions involving a derivative. We shall therefore first indicate how to replace the boundary condition (2.3.A) by a finite difference equation. By relation (5.3) of Part I we can write (2.3.A) as:

$$(2.5)\quad \frac{S_1^n - S_0^n}{h_1} - \frac{h_1}{6}\left\{ 2(S_{xx})_0^n + (S_{xx})_1^n \right\} = 0$$

and the collocation condition (2.3.C) can be written as:

$$(2.6)\quad (S_{xx})_j^n = \frac{2}{k_n}(S_j^n - S_j^{n-1}) - (S_{xx})_j^{n-1} - f_j^n - f_j^{n-1}$$

Using (2.6) in (2.5) we get

$$(2.7)\quad B_h(S_0^n, S_1^n) \equiv (-1/h_1 - 2h_1/3k_n)\, S_0^n + (1/h_1 - h_1/3k_n)\, S_1^n$$

$$+\frac{h_1}{6}\left\{\frac{4}{k_n} S_0^{n-1} + 2(S_{xx})_0^{n-1} + 2f_0^n + 2f_0^{n-1} + \frac{2}{k_n} S_1^{n-1} + (S_{xx})_1^{n-1} + f_1^n + f_1^{n-1}\right\} = 0$$

The finite difference scheme that is equivalent to the collocation scheme (2.3) is now given by

$$(2.8.\mathrm{A})\quad L_h S_j^n = 0 \qquad (1 \leq j \leq J-n-1)$$

$$(2.8.\mathrm{B})\quad B_h(S_0^n, S_1^n) = 0$$

$$(2.8.\mathrm{C})\quad S_{J-n}^n = 0$$

where $B_h(S_0^n, S_1^n)$ is defined by (2.7) and

$$L_h S_j^n = \frac{1}{3}\left\{ \frac{h_j}{h_j+h_{j+1}} \left(\frac{S_{j-1}^n - S_{j-1}^{n-1}}{k_n} \right) + 2\left(\frac{S_j^n - S_j^{n-1}}{k_n} \right) + \frac{h_{j+1}}{h_j+h_{j+1}} \left(\frac{S_{j+1}^n - S_{j+1}^{n-1}}{k_n} \right) \right\}$$

$$- \frac{1}{2}\left\{ \frac{\dfrac{S_{j+1}^n - S_j^n}{h_{j+1}} - \dfrac{S_j^n - S_{j-1}^n}{h_j}}{\frac{1}{2}(h_j+h_{j+1})} + \frac{\dfrac{S_{j+1}^{n-1} - S_j^{n-1}}{h_{j+1}} - \dfrac{S_j^{n-1} - S_{j-1}^{n-1}}{h_j}}{\frac{1}{2}(h_j+h_{j+1})} \right\}$$

$$- \frac{1}{6}\left\{ \frac{h_j}{h_j+h_{j+1}} (f_{j-1}^n + f_{j-1}^{n-1}) + 2\,(f_j^n + f_j^{n-1}) + \frac{h_{j+1}}{h_j+h_{j+1}} (f_{j+1}^n + f_{j+1}^{n-1}) \right\}$$

For the finite difference scheme (2.8) to be equivalent to the collocation scheme (2.3) it is necessary, as in Part I, to define $S^0(x)$ as the cubic spline interpolant of the initial data $g(x)$ at the meshpoints $\left\{x_j\right\}_{j=0}^{J}$. That is S^0 should satisfy

$$S_j^0 = g(x_j) \quad (0 \le j \le J)$$

with endpoint conditions

$$(S_{xx})_0^0 = g_{xx}(0)$$

and $$(S_{xx})_J^0 = g_{xx}(1)$$

{Practical computations have shown that the accuracy of the scheme is maintained and in certain cases even improved if instead we define $(S_{xx})_j^0$ by

$$(S_{xx})_j^0 = g_{xx}(x_j) \qquad (0 \leq j \leq J)\}$$

The procedure for obtaining an approximate solution to the problem (1.1) is now as follows. Suppose that the approximations to $y(x,t)$ and $y_{xx}(x,t)$ at time t_{n-1} are given by

$$\left\{S_j^{n-1}\right\}_{j=0}^{J-n+1} \quad \text{and} \quad \left\{(S_{xx})_j^{n-1}\right\}_{j=0}^{J-n+1}$$

For two distinct initial approximations $k_n^{(0)}$ and $k_n^{(1)}$ to the size of the next timestep k_n we set

$$t_n^{(0)} = t_{n-1} + k_n^{(0)}$$

and

$$t_n^{(1)} = t_{n-1} + k_n^{(1)}$$

and solve the finite difference equations (2.8), (only tridiagonal matrices are involved in the corresponding matrix equations), to obtain two sets of solution, namely

$$\left\{ S_j^{n^{(i)}} \right\}_{j=0}^{J-n} \qquad (i = 0,1)$$

From these we can explicitly compute two initial approximations to the second derivative of the solution $y(x,t)$ at the location of the approximate boundary x_{J-n}, namely

$$(2.9)\quad (S_{xx})_{J-n}^{n^{(i)}} = \frac{2}{k_n^{(i)}}\left(S_{J-n}^{n^{(i)}} - S_{J-n}^{n-1}\right) - (S_{xx})_{J-n}^{n-1} - f(x_{J-n}, t_n^{(i)}) - f_{J-n}^{n-1} \qquad (i = 0,1)$$

Similarly two initial approximations to the second derivative at the meshpoint x_{J-n-1} that is nearest to the approximate boundary x_{J-n} can be computed by

$$(2.10)\quad (S_{xx})_{J-n-1}^{n^{(i)}} = \frac{2}{k_n^{(i)}}\left(S_{J-n-1}^{n^{(i)}} - S_{J-n-1}^{n-1}\right) - (S_{xx})_{J-n-1}^{n-1} - f(x_{J-n-1}, t_n^{(i)}) - f_{J-n-1}^{n-1}$$

$$(i = 0,1)$$

Relations (2.9) and (2.10) follow from the equivalence of the collocation scheme (2.3) and the finite difference scheme (2.8). In fact these relations are a slightly rewritten form of the collocation equations (2.3c). The equivalence of the two schemes will not be shown here.

The proof requires only a minor modification of the proof following theorem 5.3 of Section I.

By making use of relation (5.2) in Lemma 5.2 of Section I, we can also get two initial approximations to the derivative of y(x,t) at the approximate boundary location x_{J-n}, namely

$$(2.11)\quad (S_x)^{n^{(i)}}_{J-n} = \frac{(S^{n^{(i)}}_{J-n} - S^{n^{(i)}}_{J-n-1})}{h_{J-n}} + \frac{h_{J-n}}{6}\left\{2(S_{xx})^{n^{(i)}}_{J-n} + (S_{xx})^{n^{(i)}}_{J-n-1}\right\}$$

$$(i = 0,1)$$

The ultimate goal is to find a zero of the function $G(k_n,S^n)$ as defined by (2.4). Since S^n depends on the choice of the timestep k_n (that is unknown beforehand) we can consider G as a function of k_n only. If we find k_n, with corresponding approximation $S^n(x)$ to the solution y(x,t) of the continuous problem (1.1) at time-level $t_{n-1}+k_n$, such that $G(k_n,S^n) = 0$ then S^n satisfies the moving boundary condition (2.2) exactly. We donnot know as yet under what conditions a root k_n of G exists, however, numerical computations have indicated that such conditions will not be too restrictive on the solutions y(x,t) and s(t) of the defining problem (1.1), apart from the fact that s(t) is assumed to be strictly decreasing with $\left|\dot{s}(t)\right| \equiv \left|\frac{ds}{dt}\right| < \infty$.

Having obtained $S^{n(0)}$ and $S^{n(1)}$ as above we now compute $G(k_n^{(0)}, S_n^{(0)})$ and $G(k_n^{(1)}, S_n^{(1)})$ where after a new approximation $k_n^{(2)}$ to k_n can be computed by for example the secant method [10, pp. 99 - 102]. That is

$$k_n^{(2)} = k_n^{(1)} - G(k_n^{(1)}, S^{n(1)}) \frac{(k_n^{(1)} - k_n^{(0)})}{G(k_n^{(1)}, S^{n(1)}) - G(k_n^{(0)}, S^{n(0)})}$$

Proceeding iteratively we get a sequence $\left\{ k_n^{(i)} \right\}_{i=0}^{m}$ and corresponding $\left\{ S^{n(i)} \right\}_{i=0}^{m}$.
The iteration is discontinued when $\left| G(k_n^{(m)}, S^{n(m)}) \right| < \epsilon$ where $\epsilon > 0$ is a pre-assigned small number. We then set

$$k_n = k_n^{(m)}$$

and

$$S_j^n = S_j^{n\,(m)} \qquad (0 \leq j \leq J-n)$$

The final approximations to the first two derivatives at the meshpoints $\left\{ x_j \right\}_{j=0}^{J-n}$ at time level t_n are again determined by

$$(2.12)\quad (S_{xx})_j^n = \frac{2}{k_n}(S_j^n - S_j^{n-1}) - (S_{xx})_j^{n-1} - f_j^n - f_j^{n-1} \qquad (0 \leq j \leq J-n-2)$$

$$(2.13)\quad (S_x)_j^n = \frac{S_{j+1}^n - S_j^n}{h_{j+1}} - \frac{h_{j+1}}{6}\left\{ 2(S_{xx})_j^n + (S_{xx})_{j+1}^n \right\} \qquad (0 \leq j \leq J-n-1)$$

$$(2.14)\quad (S_{xx})_{J-n-1}^n = (S_{xx})_{J-n-1}^{n(m)}\ ;\ (S_{xx})_{J-n}^n = (S_{xx})_{J-n}^{n(m)}\ ;\ (S_x)_{J-n}^n = (S_x)_{J-n}^{n(m)}$$

Having obtained the approximations S^n and x_{J-n} to $y(x,t_n)$ and $s(t_n)$ we can now proceed to the next time level.

III.3 Numerical Results.

The first problem is to solve

$$y_t = y_{xx} \quad (0 \leq x \leq s(t) \; ; \; 0 \leq t < \tfrac{1}{2})$$

$$y(x,0) = 1-x^2$$

$$y_x(0,t) = 0$$

$$y(s(t),t) = 0$$

$$y_x(s(t),t) - \dot{s}(t) = \frac{4t-1}{\sqrt{1-2t}}$$

which has

$$y(x,t) = 1-2t-x^2$$

and $\quad s(t) = \sqrt{1-2t}$

as its unique solution. The mesh in x-direction was taken uniform. For this problem the numerical scheme yields the exact solution. That is S_j^n, $(S_x)_j^n$, $(S_{xx})_j^n$ and x_{J-n} agree with $y(x_j,t_n)$, $y_x(x_j,t_n)$, $y_{xx}(x_j,t_n)$ and $s(t_n)$ respectively almost up to machine accuracy.
$(0 \leq j \leq J-n, \quad J > 2, \quad 1 \leq n \leq J-2)$. Also if we let $S^n(x)$ be the cubic spline interpolant of $\left\{ S_j^n \right\}_{j=0}^{J-n}$ satisfying (2.6) at x_0 and x_{J-n} then

$S^{(n)}(x)$ will be exactly equal to $y(x,t_n)$ and $x_{J-n} = s(t_n)$. (This result cannot of course, be expected in general. In this problem the simple solution is $y(x,t) = 1-2t-x^2$, which for fixed t is a polynomial of degree two in x, and for fixed x a linear function in t). The second problem is

$$y_t = y_{xx} + \frac{(-x^2-2t-1)}{\sqrt{1-2t}} \qquad (0 \leq x \leq s(t), \quad 0 \leq t < \tfrac{1}{2})$$

$$\begin{aligned} y(x,0) &= x^2-1 \\ y_x(0,t) &= 0 \\ y(s(t),t) &= 0 \\ y_x(s(t),t)\text{-}\dot{s}(t) &= 2 - 4t + \frac{1}{\sqrt{1-2t}} \end{aligned}$$

which has

$$y(x,t) = \sqrt{1-2t}\;(x^2+2t-1)$$

and

$$s(t) = \sqrt{1-2t}$$

as its unique solution. We note that $\left|\frac{ds}{dt}\right| \to \infty$ as $t \to \frac{1}{2}$.

The mesh in x-direction was taken uniform i.e.

$$h_j = x_j - x_{j-1} = h = \frac{1}{J} \qquad (1 \leq j \leq J)$$

An approximate solution was obtained with various values for J, up to time level t_N with $N = J-2$. The results are given in Table 1 with

$$e = \max \left| U_j^n - y(x_j, t_n) \right|$$

$$e_x = \max \left| (U_x)_j^n - y_x(x_j, t_n) \right|$$

$$e_{xx} = \max \left| (U_{xx})_j^n - y_{xx}(x_j, t_n) \right|$$

$$e_s = \max \left| x_{J-n} - s(t_n) \right|$$

where the maximum is taken over

$$0 \leq j \leq J-n$$

$$1 \leq n \leq N(J)$$

with $N(J)$ the largest integer such that $t_{N(J)} < .46$. For e_s (the maximum error in the approximation to the moving boundary) the maximum is taken over $0 \leq n \leq N(J)$. The quantity between brackets is the observed rate of convergence.

Table 1

e	e_x	e_{xx}	e_s	J
$.18^{-2}$ -	$.67^{-2}$ -	$.45^{-1}$ -	$.59^{-2}$ -	10 -
$.47^{-3}$ (1.95)	$.16^{-2}$ (2.0)	$.11^{-1}$ (2.0)	$.16^{-2}$ (1.90)	20
$.12^{-3}$ (2.0)	$.39^{-3}$ (2.0)	$.29^{-2}$ (1.95)	$.42^{-3}$ (1.95)	40

At each time t_{n-1} we need two initial approximations to k_n. A good approximation can be derived from (1.1.E), namely by computing

$$\gamma = \alpha^2 (s_x)^{n-1}_{J-n+1} - H(t_{n-1})$$

(γ is the approximation to $\dot{s}(t_{n-1})$)and then setting

$$k_n^{(0)} = - h_{J-n+1} / \gamma$$

$k_n^{(1)}$ can be taken as a fraction of $k_n^{(0)}$, for example take $k_n^{(1)} = 0.95\, k_n^{(0)}$. In the problem above four to five additional iterations per timestep were sufficient. (The value of $\in$ was taken to be 10^{-5}.)

For given $\mathcal{J}$ an approximate solution was computed for $N = J-2$ time levels. For larger values of J the critical time $t = \frac{1}{2}$, where the slope of the moving boundary becomes infinite, is approached more closely. Nevertheless a good accuracy was attained at time t_{J-2}, as can be seen in the table below.

Table 2

t_{J-2}	$e^{t_{J-2}}$	$e_x^{t_{J-2}}$	$e_{xx}^{t_{J-2}}$	$e_s^{t_{J-2}}$	J
.481544	$.15^{-2}$	$.11^{-1}$	$.86^{-1}$	$.79^{-2}$	10
.495398	$.24^{-3}$	$.38^{-2}$	$.56^{-1}$	$.41^{-2}$	20
.498850	$.35^{-4}$	$.11^{-2}$	$.32^{-1}$	$.20^{-2}$	40

[p. 73 does not exist]

Bibliography

[1] J. H. Ahlberg, E. N. Nilson, and J. L. Walsh; The theory of splines and their application; Academic Press; N. Y.; 1967.

[2] J. R. Cannon and C. D. Hill; Existence, uniqueness, stability and monotone dependence in a Stefan problem forrthe heat equation; J. Math. Mech.; 1 - 20; 1967.

[3] C. de Boor and B. Swartz; Collocation at Gaussian points. (To appear in SIAM J. Num. Anal.)

[4] J. Douglas Jr. and T. M. Gallie Jr.; On the numerical integration of a parabolic differential equation subject to a moving boundary condition; Duke Math. J. 22; 557 - 571; 1955.

[5] J. Douglas Jr. and T. Dupont; A finite element collocation method for non linear parabolic equations. (Manuscript).

[6] J. Douglas Jr.; Survey of numerical methods for parabolic differential equations; Advances in Computers; Vol. 2; Academic Press; N. Y.; 1961.

[7] K. W. Fong; Numerical solution of parabolic equations by the Box scheme; Thesis; California Institute of Technology; 1973.

[8] A. Friedman; Partial differential equations of parabolic type; Prentice Hall; 1964.

[9] T. N. E. Greville; ed.;Theory and applications of spline functions; Academic Press; 1969.

[10] E. Isaacson and H. B. Keller; Analysis of numerical methods; J. Wiley and Sons; N. Y.; 1966.

[11] H. B. Keller; A new difference scheme for parabolic problems; Numerical solutions of partial differential equations; Vol. 2; J. Bramble, ed.; Academic Press; N. Y.; 1971; pp. 327 - 350.

[12] G. H. Meyer; On a free interface problem for linear ordinary differential equations and the one-phase Stefan problem; Numerische Mathematik 16; 248 - 267; 1970.

[13] R. D. Russell and L. F. Shampine; A collocation method for boundary value problems; Numerische Mathematik; 1 - 28; 1972.

[14] M. H. Schultz; Spline Analysis; chapter 4; Prentice Hall; 1973.