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UNEQUALLY SPACED KNOT TECHNIQUES FOR THE

NUMERICAL SOLUTION OF PARTIAL DIFFERENTIAL EQUATIONS

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by

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ABSTRACT OF THE THESIS

"Unequally Spaced Knot Techniques for the Numerical

Solution of Partial Differential Equations"

by

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Cubic spline approximations to time dependent
partial differential equations, having both constant
and variable coefficients, are developed in which the
knot points may be chosen to be unequally spaced.
Four methods are presented for obtaining 'optimal'
knot positions, these being chosen so at to produce
an increase in accuracy compared with methods based
on equally spaced knots. Three of the procedures
described produce knot partitions which are fixed
throughout time. The fourth procedure yields
differently placed 'optimal' knots on each time line,
thus enabling us to better approximate the varying
time nature characteristic of many partial
differential equations. Truncation errors and
stability criteria are derived and full numerical
implementation procedures are given. Five case
studies are presented to enable comparisons to be
drawn between the knot placement methods and results
found using equally spaced knots. Possible extensions
of the work of this thesis are given.

CONTENTS

CHAPTER 1

Introduction

1.1   Finite Difference Solution of Partial Differential Equations

The most well-known early work on the use of finite
differences was that of Richardson (1910), although the
paper by Courant, Friedrichs and Lewy (1928) is usually
considered as the birthplace of modern numerical methods
for solving partial differential equations. In that work
Courant, Friedrichs and Lewy also showed that the
convergence of simple difference approximations depends
on the mesh ratio satisfying certain conditions. Such
conditions were also derived using Fourier techniques for
a wide variety of problems by von Neumann during the
Second World War. A detailed discussion of von Neumann's
work is given in O'Brien, Hyman and Kaplan (1951).

Since the work of von Neumann many finite difference schemes
have been proposed, perhaps the most well-known being that of
Crank and Nicolson (1947). A thorough description of methods
available is given in Richtmyer and Morton (1967). The
computational aspects and the application of finite
difference methods to partial differential equations with
variable coefficients and generalised boundary conditions
is discussed in, for example, Ames (1977), Mitchell (1969)
and Mitchell and Griffiths (1980).

The majority of finite difference schemes derived for

the solution of time dependent partial differential

equations use rectangular grids which have constant

step lengths in both the space and time directions.

There are, however, certain instances in which unequally

spaced mesh points in the space direction are beneficial.

For example, situations frequently arise in which the

solution of a partial differential equation varies very

rapidly over a small part of the domain but changes slowly

over the rest of the domain. The problem in using non-

uniform grids in such situations is that, in general, an

order of accuracy is lost by employing unequally spaced

mesh point schemes. It is therefore important to position

the mesh points so that optimal numerical performance is

achieved. Pearson (1968) proposed an iterative scheme for

the solution of boundary layer problems in which additional

mesh points are added where the variation in solution values

exceeds some predetermined level. Woodford (1975) extended

this idea and produced a scheme which used graded meshes

in which the mesh points are systematically chosen according

to the natural structure of the problem. The use of such

transformation techniques has also been considered by

various authors (see, for example, Jones and Thompson (1980)

and references therein) in determining the position of mesh

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points for the solution of fluid flow problems.

An additional area where non-uniform grids have been
used is in the numerical solution of moving boundary
problems in heat flow. Murray and Landis (1959) solved
such so-called Stefan problems by employing a uniform grid
on the solid side of the boundary and a different uniform
grid on the liquid side. A change in the size of the step
lengths therefore occurs from one side of the boundary to
the other. These moving boundary problems were also
considered by Douglas and Gallie (1955). They used a
scheme with a variable time step length which is chosen so
that the boundary always moves from one line of the space
grid to the neighbouring line in a single time step. More
recently, Crank and Gupta (1972b),proposed a method for
solving Stefan problems which employed cubic splines to
interpolate solution values.

1.2   Development of Spline Techniques

The term 'spline function' was first used by Schoenberg
(1946) in a paper describing the use of generalised splines
and other piecewise polynomials to approximate smooth
functions of one variable. Although Schoenberg's early
paper was an important contribution to the use of spline
techniques, it was not until the 1960's that further work
in the field was published.

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Since that time, spline functions have been used

extensively as methods of interpolation and approximation,

see for example, Birkhoff and de Boor (1967), Greville (1969),

Schumaker (1969), Curtis (1970), Hayes and Halliday (1974)

and Cox (1975). An excellent summary of spline techniques

is given in Ahlberg, Nilson and Walsh (1967).

Due to the benefit gained by employing splines in approximation

problems, numerous authors have adapted spline techniques to

obtain solutions to various problems in numerical analysis.

For example, Loscalzo and Talbot (1967), Loscalzo (1969),

Micula (1973) and Patricio (1978) considered the solution

of initial value problems, whilst methods for solving

two-point boundary value problems were presented by Bickley

(1968), Albasiny and Hoskins (1969), Fyfe (1969) and

Khalifa and Eilbeck (1982).

In addition, El Tom (1974 and 1976) has used spline techniques

in the solution of Volterra integral equations.

The development of spline techniques for obtaining numerical

solutions to partial differential equations began with

Papamichael and Whiteman (1973). In that work the authors

presented a method for solving the simple one-dimensional

heat conduction equation in which use was made of a cubic

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spline approximation in the space direction together with
a finite difference approximation in the time direction.
A similar technique was used by Raggett and Wilson (1974)
in obtaining numerical solutions to the one-dimensional
wave equation.

Spline function approximations have since been applied
to more general partial differential equations. For example,
Raggett, Stone and Wisher (1976) considered the solution
of practical problems modelled by hyperbolic partial
differential equations of the form

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x}\left[a(x,t)\frac{\partial u}{\partial x}\right] + b(x,t)\frac{\partial u}{\partial x} + c(x,t)u. \quad (1.2.1)$$

In addition, Rubin and Graves (1975) and Rubin and Khosla
(1976) presented spline techniques for solving problems in
fluid mechanics. In particular, their work developed the
use of spline techniques in the solution of non-linear
equations. The application of spline function approximations
to partial differential equations in two space dimensions
was considered by Jain and Holla (1978). They proposed a
high accuracy formula, using a technique similar to that
of McKee (1973), for the spline solution of wave equations of

the form

$$\frac{\partial^2 u}{\partial t^2} = a(x,y,t) \frac{\partial^2 u}{\partial x^2} + b(x,y,t) \frac{\partial^2 u}{\partial y^2} \ . \qquad (1.2.2)$$

Jain and Aziz (1981) have also recently applied parametric

spline techniques to a variety of differential equations and

have found that they compare favourably with the more usual

cubic spline approximations. In addition, papers by Sastry

(1976) and Pala and Spano (1978) have also proposed methods

for obtaining spline solutions to parabolic partial

differential equations.

1.3   Motivation for Present Work

As mentioned earlier, the use of cubic splines for the

numerical solution of the one-dimensional wave equation

has been considered by Raggett and Wilson (1974). An

indication of how that work could be generalised to the

solution of more general one-dimensional, constant coefficient,

hyperbolic partial differential equations was shown by

Raggett (1974). The completion of that work was carried

out by Wisher (1977), who indicated that the use of spline

techniques gave increased accuracy over comparative

finite difference approximations. The schemes used on

hyperbolic equations by Wisher (1977) are illustrated in Chapter 3 of this thesis. The extension of that work to include parabolic partial differential equations is also given in Chapter 3.

Most of the previously mentioned works on the application of spline techniques to the solution of partial differential equations have produced methods in which the knots were chosen to be equally spaced. An exception here is that of Wisher (1977) who used unequally spaced knots in solving the simple wave equation. In that work, the knots were positioned in an ad-hoc manner and no improvement in accuracy was observed over the use of uniform knot partitions. Further, some experimentation on choosing the knot points to be the zeros or extrema of the shifted Chebyshev polynomial

$$T_n^*(x) = \cos(n\cos^{-1}(2x-1)) \qquad\qquad (1.2.3)$$

was undertaken in Wisher (1977). Again no improvement in accuracy over constant knot spacing was observed.

In this thesis we employ spline techniques with unequally spaced knots for the numerical solution of both hyperbolic and parabolic partial differential equations. Further, we present methods for the optimal positioning of these knots.

The derivation of schemes allowing the non-uniform partitioning
of knot points is given in Chapter 4.

The problem of determining optimal positions of knots
has been shown to be a difficult one and has only to-date
been applied to approximation problems.

In the earlier works on approximating functions (see for
example, Curtis and Powell (1967)) equally spaced knots
were employed with additional knots being inserted when
the error in the approximation was larger than some
prescribed magnitude. Since that time various authors
have attempted to choose the positions of the knots, in
some optimal sense, given knowledge about the function f
being approximated. De Boor and Rice (1968) described an
algorithm for solving the least-squares cubic spline
approximation problem. Their idea was to vary one knot
at a time so as to reduce the error of best approximation.
Similarly, Esch and Eastman (1969) proposed a method for
a best discrete Chebyshev approximation by splines. Both
these algorithms are computationally expensive and de Boor
(1973) has since proposed an alternative method which chooses
the knot partition from the given function f. This method
is applied to the solution of partial differential equations

in Chapter 5 by taking the function f to be the given

initial condition. Two additional methods for optimally

positioning the knots are also derived in Chapter 5.

In Chapter 6 of this thesis, a number of case studies

are considered and solutions derived using knot partitions

resulting from each of the methods given in Chapter 5.

Comparisons are also made with results produced using equally

spaced knots.

The results of Chapter 6 suggest that improvement on the

methods for locating the knot points given in Chapter 5 would

be desirable. An improved algorithm is thus presented in

Chapter 7, which chooses optimal partitions of knots on each

time line. The suitability of this method is examined in

Chapter 8, where the earlier case studies are again considered.

Throughout this thesis, no particular reference to the

associated characteristics has been made for hyperbolic

problems. However, it should be realised that due

account has been taken in the satisfaction of the

Courant Friedrichs Lewy condition (see Mitchell and

Griffiths (1980)) for all the problems cited.

CHAPTER 2

Review of Cubic Spline Theory

2.1   Definition of a Cubic Spline

Let f(x) be a function with continuous derivatives in

the range $a \leqslant x \leqslant b$. To approximate f(x) using cubic

spline techniques we may subdivide the interval $a \leqslant x \leqslant b$

into N sub-intervals by inserting knots x_i such that

$$a = x_0 < x_1 < ....< x_N = b. \qquad (2.1.1)$$

S(x) is a cubic spline interpolating to the function f(x) at

the knots x_0, x_1,.....,x_N if

(i)   in each sub-interval $x_{i-1} \leqslant x \leqslant x_i$ (i=1,2,...,N),

        S(x) is a cubic polynomial,

(ii) $S'(x)$ and $S''(x)$ are continuous everywhere in $\left[a,b\right]$,

(iii) $S(x_i) = f(x_i)$ (i=0,1,...,N).

A cubic spline thus consists of a set of cubic polynomial

arcs which are joined smoothly end to end with continuous

first and second derivatives. In general, the third derivative

will have a discontinuity at each of the knots $x_1, x_2,.....,x_{N-1}$.

2.2   Cubic Spline Functions

From Ahlberg, Nilson and Walsh (1967), in the interval

$\left[x_{i-1}, x_i\right]$ we define $S''(x)$ as

$$S''(x) = M_{i-1} \left(\frac{x_i - x}{h_i} \right) + M_i \left(\frac{x - x_{i-1}}{h_i} \right) \qquad (2.2.1)$$

where $\quad h_i = x_i - x_{i-1} \quad (i = 1,2,\ldots,N)$ $\qquad$ (2.2.2)

and $M_i = S''(x_i)$. Integrating twice gives the cubic spline

function $S(x)$ on $\left[x_{i-1}, x_i \right]$ as

$$S(x) = M_{i-1} \frac{(x_i - x)^3}{6h_i} + M_i \frac{(x - x_{i-1})^3}{6h_i} + \left(f(x_{i-1}) - \frac{h_i^2}{6} M_{i-1} \right) \frac{(x_i - x)}{h_i}$$

$$+ \left(f(x_i) - \frac{h_i^2}{6} M_i \right) \frac{(x - x_{i-1})}{h_i} \quad (i=1,2,\ldots,N)$$

$$\qquad (2.2.3)$$

the constants of integration being evaluated from $S(x_i) = f(x_i)$

and $S(x_{i-1}) = f(x_{i-1})$. From (2.2.3) the following one-sided

limits of the derivatives of $S'(x)$ are derived

$$S'(x_i-) = \frac{h_i}{6} M_{i-1} + \frac{h_i}{3} M_i + \frac{f(x_i) - f(x_{i-1})}{h_i} \quad (i=1,2,\ldots,N)$$

$$\qquad (2.2.4)$$

$$S'(x_i+) = -\frac{h_{i+1}}{3} M_i - \frac{h_{i+1}}{6} M_{i+1} + \frac{f(x_{i+1}) - f(x_i)}{h_{i+1}} \quad (i=0,1,\ldots(N-1))$$

$$\qquad (2.2.5)$$

The unknowns $M_i (i=0,2,\ldots,N)$ are obtained by equating these

one-sided limits, thus giving

$$\frac{h_i}{6} M_{i-1} + \frac{h_i + h_{i+1}}{3} M_i + \frac{h_{i+1}}{6} M_{i+1} = \frac{h_i f(x_{i+1}) - (h_i + h_{i+1}) f(x_i) + h_{i+1} f(x_{i-1})}{h_i h_{i+1}}$$

$$(i=1,2,\ldots,(N-1))$$

$$\qquad (2.2.6)$$

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Equation (2.2.6) is a tri-diagonal system of (N-1)

equations in (N+1) unknowns. To solve this system various

choices of conditions are available at the end points,

x_0 and x_N, of the interval to produce a consistent set

of (N+1) equations

(i) $S''(x_i) = 0$ (i=0,N)   (2.2.7)

(ii) $S'(x_i) = f'(x_i)$ (i=0,N)   (2.2.8)

(III) $S''(x_i) = f''(x_i)$ (i=0,N)   (2.2.9)

As suggested by Behforooz and Papamichael (1979), the

choice of these extra conditions plays an important role

on the quality of the spline approximation. It is well-known

that the best order of approximation which can be achieved

by an interpolatory cubic spline is

$$|| S - f || = O(h^4)$$

where $|| . ||$ denotes the uniform norm on $[a,b]$ and

$h = \max(h_i)$. This order of accuracy is obtained if either

(ii) or (iii) are used as the extra conditions. As stated

by Kershaw (1973) an $O(h^4)$ accuracy is not obtained if

condition (i) is applied. However, the conditions (ii)

and (iii) require knowledge of the derivatives of the

function f(x). This knowledge is not generally available

from any imposed boundary conditions of partial differential

equations and we thus use (i) as the extra conditions in

this thesis, S(x) and (i) being known as a 'natural'

cubic spline. Papamichael and Worsey (1981) have

recently derived improved extra conditions for spline

approximation which could result in increased accuracy

to the results of case studies considered later.

Having decided on the choice of 'end conditions', substitution

of these into (2.2.6) gives a system of (N-1) equations which

are linearly independent, tri-diagonal and diagonally

dominant. They can therefore easily be solved for M_i

(i=1,2,...,(N-1)), the satisfaction of the end conditions

then giving M_0 and M_N. The spline function S(x) can then

be obtained from (2.2.3).

CHAPTER 3

Initial Value Partial Differential Equations with Equally Spaced Knots.

(i)   Hyperbolic Partial Differential Equations

3.1   Constants Coefficients

Suppose that $u(x,t)$ satisfies the second order linear hyperbolic partial differential equation

$$\frac{\partial^2 u}{\partial t^2} = a\frac{\partial^2 u}{\partial x^2} + b\frac{\partial u}{dx} + cu \quad (0 \leqslant x \leqslant 1, \; t > 0) \qquad (3.1.1)$$

where the coefficients a, b, c are constants $(a > 0)$.

Assume further that (3.1.1) is subject to the function value boundary conditions

$$u(0,t) = f_1(t) \quad , \quad u(1,t) = f_2(t) \qquad (3.1.2)$$

and the initial conditions

$$u(x,0) = g_1(x) \quad , \quad \frac{\partial u(x,0)}{\partial t} = g_2(x) \qquad (3.1.3)$$

where $f_1(t)$, $f_2(t)$, $g_1(x)$ and $g_2(x)$ are known functions.

To obtain solutions to (3.1.1) using spline techniques we here consider the knots

$$0 = x_0 < x_1 < \ldots < x_N = 1 \qquad (3.1.4)$$

to be equally spaced where the distance between successive knots is h, so that $x_i = ih$ $(i=0,1,\ldots,N)$. We now replace the time derivative in (3.1.1) by a finite difference approximation and the space derivatives by a cubic spline, thus obtaining at the point (ih, jk) the implicit relationship (see Wisher (1977))

$$\frac{u_{i,j-1}-2u_{i,j}+u_{i,j+1}}{k^2} = a\left\{\theta M_{i,j-1}+(1-2\theta)M_{i,j}+\theta M_{i,j+1}\right\}$$

$$+ b\left\{\theta L_{i,j-1}+(1-2\theta)L_{i,j}+\theta L_{i,j+1}\right\}$$

$$+ c\left\{\theta u_{i,j-1}+(1-2\theta)u_{i,j}+\theta u_{i,j+1}\right\} \qquad (3.1.5)$$

$(i=0,1,\ldots,N;\; j=1,2,\ldots;\; Nh=1\;;\; \theta \geqslant 0)$

where $L_{i,j} = S_j'(x_i)$, $M_{i,j} = S_j''(x_i)$; $S_j(x)$ denoting the cubic spline interpolating the values $u_{i,j}$ on the jth time line, this being given by

$$S_j(x) = M_{i-1,j}\frac{(x_i-x)^3}{6h} + M_{i,j}\frac{(x-x_{i-1})^3}{6h} + \left(u_{i-1,j}-\frac{h^2}{6}M_{i-1,j}\right)\frac{(x_i-x)}{h}$$

$$+ \left(u_{i,j}-\frac{h^2}{6}M_{i,j}\right)\frac{(x-x_{i-1})}{h} \qquad (i=1,2,\ldots,N)\ (3.1.6)$$

As shown in section 2.2, the continuity of the first derivatives of the spline function yields

$$\frac{1}{6}M_{i-1,j} + \frac{2}{3}M_{i,j} + \frac{1}{6}M_{i+1,j} = \frac{u_{i-1,j}-2u_{i,j}+u_{i+1,j}}{h^2} \qquad (3.1.7)$$

$$(i=1,2,\ldots,(N-1))$$

This relationship also holds on the $(j-1)^{th}$ and $(j+1)^{th}$ time lines, giving respectively

$$\frac{1}{6}M_{i-1,j-1}+ \frac{2}{3}M_{i,j-1}+ \frac{1}{6}M_{i+1,j-1} = \frac{u_{i-1,j-1}-2u_{i,j-1}+u_{i+1,j-1}}{h^2}$$

$$(i=1,2,\ldots,(N-1))$$

$$(3.1.8)$$

and

$$\frac{1}{6}M_{i-1,j+1} + \frac{2}{3}M_{i,j+1} + \frac{1}{6}M_{i+1,j+1} = \frac{u_{i-1,j+1}-2u_{i,j+1}+u_{i+1,j+1}}{h^2}$$

$$(i=1,2,\ldots,(N-1))$$

$$(3.1.9)$$

We now require an expression similar to (3.1.7) which incorporates the $L_{i,j}$ values. On the jth time line (2.2.4) and (2.2.5) respectively become

$$L_{i,j} = S_j'(x_i-) = \frac{hM}{6}_{i-1,j} + \frac{hM}{3}_{i,j} + \frac{u_{i,j} - u_{i-1,j}}{h} \qquad (3.1.10)$$

$$(i=1,2,\ldots,N)$$

and

$$L_{i,j} = S_j'(x_i+) = \frac{-hM}{3}_{i,j} \frac{-hM}{6}_{i+1,j} + \frac{u_{i+1,j} - u_{i,j}}{h} \qquad (3.1.11)$$

$$(i=0,1,\ldots,(N-1))$$

From (3.1.10) we have

$$L_{i+1,j} = \frac{hM}{6}_{i,j} + \frac{hM}{3}_{i+1,j} + \frac{u_{i+1,j} - u_{i,j}}{h} \qquad (3.1.12)$$

$$(i=0,1,\ldots,(N-1))$$

and from (3.1.11)

$$L_{i-1,j} = \frac{-hM}{3}_{i-1,j} - \frac{hM}{6}_{i,j} + \frac{u_{i,j} - u_{i-1,j}}{h} \qquad (3.1.13)$$

$$(i=1,2,\ldots,N)$$

A relationship is now obtained by adding (3.1.10) and (3.1.11), the result being added to half the sum of (3.1.12) and (3.1.13). Thus on the jth time line

$$\frac{1}{6}L_{i-1,j} + \frac{2}{3}L_{i,j} + \frac{1}{6}L_{i+1,j} = \frac{u_{i+1,j} - u_{i-1,j}}{2h} \qquad (3.1.14)$$

$$(i=1,2,\ldots,(N-1))$$

Again (3.1.14) holds on the $(j-1)^{th}$ and $(j+1)^{th}$ time lines giving

$$\frac{1}{6}L_{i-1,j-1} + \frac{2}{3}L_{i,j-1} + \frac{1}{6}L_{i+1,j-1} = \frac{u_{i+1,j-1} - u_{i-1,j-1}}{2h} \qquad (3.1.15)$$

$$(i=1,2,\ldots,(N-1))$$

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and

$$\frac{1}{6}L_{i-1,j+1} + \frac{2}{3}L_{i,j+1} + \frac{1}{6}L_{i+1,j+1} = \frac{u_{i+1,j+1} - u_{i-1,j+1}}{2h} \quad (3.1.16)$$

$$(i=1,2,....,(N-1))$$

As shown in Wisher (1977) the required scheme incorporating splines is obtained by performing the following operations:

(i) multiply (3.1.7) by $a(1-2\theta)$;

(ii) add (3.1.8) and (3.1.9), multiply the result by $a\theta$;

(iii) multiply (3.1.14) by $b(1-2\theta)$;

(iv) add (3.1.15) and (3.1.16), multiply the result by $b\theta$;

(v) add the expressions produced in (i) - (iv) together;

(vi) use (3.1.5) to eliminate the $M_{i,j}$ and $L_{i,j}$ values,

thus giving the following three time level scheme

$$(1-\beta_1\theta)u_{i-1,j+1} + 4(1+\beta_2\theta)u_{i,j+1} + (1-\beta_3\theta)u_{i+1,j+1}$$

$$=\{2+\beta_1(1-2\theta)\}\, u_{i-1,j} + 4\{2-\beta_2(1-2\theta)\}\, u_{i,j} + \{2+\beta_3(1-2\theta)\}\, u_{i+1,j}$$

$$-(1-\beta_1\theta)u_{i-1,j-1} - 4(1+\beta_2\theta)u_{i,j-1} - (1-\beta_3\theta)u_{i+1,j-1} \quad (3.1.17)$$

$$(i=1,2,....,(N-1))$$

where $\beta_1 = 6ar^2-3brk+ck^2$; $\beta_2=3ar^2-ck^2$; $\beta_3=6ar^2+3brk+ck^2$

and the mesh ratio $r=k/h$.

The truncation error for (3.1.17) is obtained by expanding each term of the scheme about the mesh point (ih,jk) using Taylor series approximations. After appropriate rearrangements (see Wisher (1977)) the following expression, to fourth order, is obtained

$$k^2h^2 \left[c^2r^2f(\theta)u + 2bcr^2f(\theta)\frac{\partial u}{\partial x} \right.$$

$$+ \left\{ r^2(2ac + b^2)f(\theta) - \frac{1}{6} c^2k^2\theta \right\} \frac{\partial^2 u}{\partial x^2}$$

$$+ \left\{ 2abr^2f(\theta) - \frac{1}{6} bck^2\theta \right\} \frac{\partial^3 u}{\partial x^3}$$

$$+ \left. \left\{ a^2r^2f(\theta) + \frac{1}{12} a - \frac{1}{72} ch^2 - \frac{1}{6} ack^2\theta \right\} \frac{\partial^4 u}{\partial x^4} \right] \tag{3.1.18}$$

where $\quad f(\theta) = \frac{1}{12}(1 - ck^2\theta) - \theta. \tag{3.1.19}$

This truncation error may be considerably simplified by choosing $f(\theta) = 0$, in which case the parameter θ is chosen such that

$$\theta = \frac{1}{12 + ck^2} \tag{3.1.20}$$

Thus, in the special case where fourth and higher order derivatives are small, the truncation error is reduced in magnitude from $O(k^2h^2)$ to $O(k^4h^2)$. The technique of optimally choosing the parameter θ has been considered in detail by Wisher (1977). For example, when obtaining solutions to the wave equation ((3.1.1) with a=1, b=c=0) the truncation error (3.1.18) can be reduced to $O(k^2h^4+k^6)$ by choosing

$$\theta = \frac{1}{12r^2}(1+r^2) \tag{3.1.21}$$

and, in fact, to $O(k^2h^6+k^8)$ by suitable choice of both θ and r.

To examine the stability of the scheme (3.1.17) we use the well known von Neumann method (see Mitchell (1969)) in which a harmonic decomposition is made of the error at mesh points (see Wisher (1977) for full details). The following stability conditions are obtained

(a) if $\theta \geqslant \frac{1}{4}$, it is unconditionally stable

(b) if $\theta < \frac{1}{4}$, it is stable when

$$r \leqslant \{3a(1-4\theta)\}^{-1/2} \; . \qquad (3.1.22)$$

3.2   Variable Coefficients.

Here we require solutions to the hyperbolic partial differential equation

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x}\left[a(x,t)\, \frac{\partial u}{\partial x} \right] + b(x,t)\, \frac{\partial u}{\partial x} + c(x,t)u \qquad (3.2.1)$$

where $a(x,t)$, $b(x,t)$ and $c(x,t)$ are variable coefficients and $a(x,t) > 0$ at all points in the solution domain. Again we consider the knots to be equally spaced and perform an analysis identical to that of the previous section. Though complicated by the variable coefficients the following scheme, similar to (3.1.17), is derived at (ih,jk)

$$(\phi_{i-1,j+1} - \theta\psi_{i,j+1})u_{i-1,j+1} + 4(\phi_{i,j+1} + 3\gamma_{i,j+1})u_{i,j+1}$$

$$+(\phi_{i+1,j+1} - \theta\chi_{i,j+1})u_{i+1,j+1}$$

$$=\{2\phi_{i-1,j} + k^2 c_{i-1,j} + (1-2\theta)\psi_{i,j}\} u_{i-1,j} + 4\{2\phi_{i,j} + k^2 c_{i,j}$$

$$-3(1-2\theta)\gamma_{i,j}\} u_{ij} + \{2\phi_{i+1,j} + k^2 c_{i+1,j} + (1-2\theta)\chi_{i,j}\} u_{i+1,j}$$

$$- (\phi_{i-1,j-1} - \theta\psi_{i,j-1})u_{i-1,j-1} -4(\phi_{i,j-1} + 3\gamma_{i,j-1})u_{i,j-1}$$

$$-(\phi_{i+1,j-1} - \theta\chi_{i,j-1})u_{i+1,j-1} \qquad (i=1,2,\ldots,(N-1)) \qquad (3.2.2)$$

where

$$\phi_{i,j} = 1 - k^2\theta c_{i,j} \ , \ \gamma_{i,j} = r^2 a_{i,j} \ , \ \psi_{i,j} = 6\gamma_{i,j} - \beta_{i,j} \ ,$$

$$\chi_{i,j} = 6\gamma_{i,j} + \beta_{i,j} \ , \ \beta_{i,j} = 3rk(a'_{i,j} + b_{i,j}) \ ,$$

the prime denoting differentiation with respect to x.

The truncation error for (3.2.2) is again obtained using Taylor series expansions. It is found that the error is $O(k^2 h^2)$, although in this case the expression is much more complex, involving derivatives of the variable coefficients and odd order derivatives of u with respect to t. The full expression for this truncation error is given in Wisher (1977).

The stability condition for (3.2.2) is obtained by applying the von Neumann method locally, since the method is only applicable to difference schemes with constant coefficients.

As suggested by Widlund (1966) and Mitchell (1969) we therefore perform the analysis by considering the coefficients to be constant and assume that the scheme with variable coefficients will be stable provided the condition obtained is satisfied at every point of the solution domain. The scheme (3.2.2) then has the following stability condition

(a)   if $\theta \geq \frac{1}{4}$, it is unconditionally stable;

(b)   if $\theta < \frac{1}{4}$, it is stable whenever

$$r \leq \{3a(x,t)(1-4\theta)\}^{-1/2} \qquad (3.2.3)$$

is satisfied independently at each point of the solution domain.

Equations of the form (3.2.1) have been considered in detail by Raggett, Stone and Wisher (1975) and (1976).

(ii)   **Parabolic Partial Differential Equations**

3.3   **Constant Coefficients**

The cubic spline solution of the simple heat conduction equation has been considered by Papamichael and Whiteman(1973) and by Sastry (1976). In this section we extend the technique to the more general parabolic partial differential equation

$$\frac{\partial u}{\partial t} = a \frac{\partial^2 u}{\partial x^2} + b \frac{\partial u}{\partial x} + cu \qquad (0 \leq x \leq 1, \ t > 0) \qquad (3.3.1)$$

where a, b, c are constants ($a > 0$). We here assume that

(3.3.1) is subject to the initial condition

$$u(x,0) = g(x) \qquad\qquad (3.3.2)$$

and the function value boundary conditions

$$u(0,t) = f_1(t) \quad , \quad u(1,t) = f_2(t) \qquad\qquad (3.3.3)$$

Where $f_1(t)$, $f_2(t)$ and $g(x)$ are known functions. If the

knot partition (3.1.4) is again chosen to be equally spaced,

then by similarly replacing the time derivative in (3.3.1)

by a finite difference approximation and the space derivatives

by a cubic spline we have at (ih,jk)

$$\frac{u_{i,j+1} - u_{i,j}}{k} = a\{\theta M_{i,j+1} + (1-\theta)M_{i,j}\}$$

$$+ b\{\theta L_{i,j+1} + (1-\theta)L_{i,j}\}$$

$$+ c\{\theta u_{i,j+1} + (1-\theta)u_{i,j}\} \qquad (3.3.4)$$

(i=0,1,.....,N ; j=1,2,.... ; Nh=1 ; $\theta \geqslant 0$)

where $L_{i,j}$ and $M_{i,j}$ are as previously defined. A scheme

similar in nature to (3.1.17) is obtained by performing the

following operations:

(i)   multiply (3.1.7) by $a(1-\theta)$;

(ii)   multiply (3.1.9) by $a\theta$;

(iii)   multiply (3.1.14) by $b(1-\theta)$;

(iv)   multiply (3.1.16) by $b\theta$;

(v)   add the expressions produced in (i)-(iv) above

together;

(vi)   use (3.3.4) to eliminate the $M_{i,j}$ and $L_{i,j}$ values.

The following scheme incorporating splines thus results

$$(1-\beta_1\theta)u_{i-1,j+1} + 4(1+\beta_2\theta)u_{i,j+1} + (1-\beta_3\theta)u_{i+1,j+1}$$

$$= \{1+\beta_1(1-\theta)\}u_{i-1,j} + 4\{1-\beta_2(1-\theta)\}u_{i,j} + \{1+\beta_3(1-\theta)\}u_{i+1,j} \quad (3.3.5)$$

$$(i=1,2,\ldots,(N-1))$$

where $\beta_1 = 6ar - 3brh + kc$; $\beta_2 = 3ar - ck$; $\beta_3 = 6ar + 3brh + kc$
and the mesh ratio $r = k/h^2$.

The scheme (3.3.5) reduces to that of Papamichael and

Whiteman (1973) for $a=1$, $b=c=0$ and is analogous to (3.1.17)

for hyperbolic equations. In fact, if $a=1$, $b=c=0$, suitable

choices of the parameter θ lead to other well-known finite

difference schemes. For example, by choosing $\theta = \dfrac{1}{6r}$ the

scheme (3.3.5) reduces to the simple explicit representation;

$\theta = \dfrac{1}{2} + \dfrac{1}{6r}$ gives rise to the Crank-Nicolson formula and

$\theta = \dfrac{1}{2} + \dfrac{1}{12r}$ yields the high accuracy formula of Douglas

(1956).

The truncation error associated with the scheme (3.3.5) is again obtained using Taylor series expansions. Fuller details are given here (compared to the hyperbolic case) since this truncation error has not been derived elsewhere. Thus, expanding (3.3.5) about the mesh point (ih, jk) we have

$$(1-\beta_1\theta)\left[u_{i,j} + k\left(\frac{\partial u}{\partial t}\right)_{i,j} + \frac{k^2}{2!}\left(\frac{\partial^2 u}{\partial t^2}\right)_{i,j} + \frac{k^3}{3!}\left(\frac{\partial^3 u}{\partial t^3}\right)_{i,j} + \frac{k^4}{4!}\left(\frac{\partial^4 u}{\partial t^4}\right)_{i,j}\right.$$

$$-h\left\{\left(\frac{\partial u}{\partial x}\right)_{i,j} + k\left(\frac{\partial^2 u}{\partial x\partial t}\right)_{i,j} + \frac{k^2}{2!}\left(\frac{\partial^3 u}{\partial x\partial t^2}\right)_{i,j} + \frac{k^3}{3!}\left(\frac{\partial^4 u}{\partial x\partial t^3}\right)_{i,j}\right\}$$

$$+\frac{h^2}{2!}\left\{\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} + k\left(\frac{\partial^3 u}{\partial x^2\partial t}\right)_{i,j} + \frac{k^2}{2!}\left(\frac{\partial^4 u}{\partial x^2\partial t^2}\right)_{i,j}\right\}$$

$$\left. -\frac{h^3}{3!}\left\{\left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j} + k\left(\frac{\partial^4 u}{\partial x^3\partial t}\right)_{i,j}\right\} + \frac{h^4}{4!}\left(\frac{\partial^4 u}{\partial x^4}\right)_{i,j}\right]$$

$$+ 4(1-\beta_2\theta)\left[u_{i,j} + k\left(\frac{\partial u}{\partial t}\right)_{i,j} + \frac{k^2}{2!}\left(\frac{\partial^2 u}{\partial t^2}\right)_{i,j} + \frac{k^3}{3!}\left(\frac{\partial^3 u}{\partial t^3}\right)_{i,j} + \frac{k^4}{4!}\left(\frac{\partial^4 u}{\partial t^4}\right)_{i,j}\right]$$

$$+(1-\beta_3\theta)\left[u_{i,j} + k\left(\frac{\partial u}{\partial t}\right)_{i,j} + \frac{k^2}{2!}\left(\frac{\partial^2 u}{\partial t^2}\right)_{i,j} + \frac{k^3}{3!}\left(\frac{\partial^3 u}{\partial t^3}\right)_{i,j} + \frac{k^4}{4!}\left(\frac{\partial^4 u}{\partial t^4}\right)_{i,j}\right.$$

$$+h\left\{\left(\frac{\partial u}{\partial x}\right)_{i,j} + k\left(\frac{\partial^2 u}{\partial x\partial t}\right)_{i,j} + \frac{k^2}{2!}\left(\frac{\partial^3 u}{\partial x\partial t^2}\right)_{i,j} + \frac{k^3}{3!}\left(\frac{\partial^4 u}{\partial x\partial t^3}\right)_{i,j}\right\}$$

$$+\frac{h^2}{2!}\left\{\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} + k\left(\frac{\partial^3 u}{\partial x^2\partial t}\right)_{i,j} + \frac{k^2}{2!}\left(\frac{\partial^4 u}{\partial x^2\partial t^2}\right)_{i,j}\right\}$$

$$\left. +\frac{h^3}{3!}\left\{\left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j} + k\left(\frac{\partial^4 u}{\partial x^3\partial t}\right)_{i,j}\right\} + \frac{h^4}{4!}\left(\frac{\partial^4 u}{\partial x^4}\right)_{i,j}\right]$$

$$= \{1+\beta_1(1-\theta)\} \left[u_{i,j} - h \left(\frac{\partial u}{\partial x}\right)_{i,j} + \frac{h^2}{2!} \left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} - \frac{h^3}{3!} \left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j} + \frac{h^4}{4!} \left(\frac{\partial^4 u}{\partial x^4}\right)_{i,j} \right]$$

$$+ 4 \{1-\beta_2(1-\theta)\} u_{i,j}$$

$$+ \{1+\beta_3(1-\theta)\} \left[u_{i,j} + h \left(\frac{\partial u}{\partial x}\right)_{i,j} + \frac{h^2}{2!} \left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} + \frac{h^3}{3!} \left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j} + \frac{h^4}{4!} \left(\frac{\partial^4 u}{\partial x^4}\right)_{i.j} \right]$$

$$(3.3.6)$$

Using the expressions for β_1, β_2, β_3 given earlier and rearranging we obtain the following truncation error to fourth order

$$(-ck^2\theta) \frac{\partial u}{\partial t} + \frac{1}{2} (k^2 - ck^3\theta) \frac{\partial^2 u}{\partial t^2} + \frac{1}{6} (k^3 - ck^4\theta) \frac{\partial^3 u}{\partial t^3}$$

$$+ \frac{1}{24} (k^4 - ck^5\theta) \frac{\partial^4 u}{\partial t^4} + (-bk^2\theta) \frac{\partial^2 u}{\partial x \partial t} + (- \frac{1}{2}bk^3\theta) \frac{\partial^3 u}{\partial x \partial t^2}$$

$$+ (- \frac{1}{6}bk^4\theta) \frac{\partial^4 u}{\partial x \partial t^3} + (- \frac{1}{6}ckh^2) \frac{\partial^2 u}{\partial x^2} + \frac{1}{6} (kh^2 - 6ak^2\theta - ck^2h^2\theta) \frac{\partial^4 u}{\partial x^2 \partial t^2}$$

$$+ \frac{1}{6} (\frac{k^2h^2}{12} - 3ak^3\theta - \frac{ck^3h^2}{2}\theta) \frac{\partial^4 u}{\partial x^2 \partial t^2} + (- \frac{1}{6}bkh^2) \frac{\partial^3 u}{\partial x^3}$$

$$+ (- \frac{1}{6}bk^2h^2\theta) \frac{\partial^4 u}{\partial x^3 \partial t} + \frac{1}{12} \left(-akh^2 - \frac{ckh^4}{6}\right) \frac{\partial^4 u}{\partial x^4} \qquad (3.3.7)$$

The time and mixed derivatives in (3.3.7) can now be replaced by space derivatives by employing (3.3.1).

For example

$$\frac{\partial^2 u}{\partial t^2} = a^2 \frac{\partial^4 u}{\partial x^4} + 2ab \frac{\partial^3 u}{\partial x^3} + (2ac + b^2) \frac{\partial^2 u}{\partial x^2} + 2bc \frac{\partial u}{\partial x} + c^2 u,$$

$$\frac{\partial^2 u}{\partial x \partial t} = a \frac{\partial^3 u}{\partial x^3} + b \frac{\partial^2 u}{\partial x^2} + c \frac{\partial u}{\partial x} \quad .$$

The following expression for the truncation error

involving space derivatives only, is thus obtained

$$
k^2 \left\{ \left[c^2 \left(\frac{1}{2}(1-2\theta) + \frac{ck}{6}(1-3\theta) + \frac{c^2 k^2}{24}(1 - 4\theta - ck\theta) \right) \right] u \right.
$$

$$
+ \left[bc \left(1-2\theta + \frac{ck}{2}(1-3\theta) + \frac{c^2 k^2}{6}(1 - 4\theta - ck\theta) \right) \right] \frac{\partial u}{\partial x}
$$

$$
+ \left[ac \left(1-2\theta + \frac{ck}{2}(1-3\theta) + \frac{c^2 k^2}{6}(1 - 3\theta - ck\theta) \right) \right.
$$

$$
+ b^2 \left(\frac{1}{2}(1-2\theta) + \frac{ck}{2}(1-3\theta) + \frac{c^2 k^4}{4}(1 - 4\theta - ck\theta) \right)
$$

$$
\left. + \frac{c^2 h^2}{72} (1 - 12\theta - ck\theta) \right] \frac{\partial^2 u}{\partial x^2}
$$

$$
+ \left[ab \left(1-2\theta + ck(1-3\theta) + \frac{c^2 k^2}{2}(1 - 3\theta - ck\theta) \right) \right.
$$

$$
+ b^3 \left(\frac{ck^2}{6}(1 - 4\theta - ck\theta) + \frac{k}{6}(1 - 3\theta) \right)
$$

$$
\left. + \frac{bch^2}{36} (1 - 12\theta - 6ck\theta) \right] \frac{\partial^3 u}{\partial x^3}
$$

$$
+ \left[a^2 \left(\frac{1}{2}(1-2\theta) + \frac{ck}{2}(1-3\theta) + \frac{c^2 k^2}{4}(1-2\theta - ck\theta) \right) \right.
$$

$$
+ ab^2 \left(\frac{k}{2}(1-3\theta) + \frac{ck^2}{2}(1 - 3\theta - ck\theta) \right)
$$

$$
+ \frac{ach^2}{36} (1 - 6\theta - 6ck\theta) + \frac{b^2 h^2}{72} (1 - 12\theta - 6ck\theta)
$$

$$
\left. + \frac{b^4 k^2}{24} (1 - 4\theta - ck\theta) + \frac{a}{12r} - \frac{ch^2}{72r} \right] \frac{\partial^4 u}{\partial x^4} \right\} \tag{3.3.8}
$$

For the simple heat conduction equation this error
reduces to

$$k^2 \left[\frac{1}{2}(1-2\theta) + \frac{1}{12r} \right] \frac{\partial^4 u}{\partial x^4} \quad + \dots \quad (3.3.9)$$

and thus by choosing

$$\theta = \frac{1}{2} + \frac{1}{12r} \quad\quad (3.3.10)$$

the truncation error is simplified to include only terms

higher than fourth order derivatives. As previously mentioned,

the use of (3.3.10) gives rise to the high accuracy formula

derived by Douglas (1956).

The stability of (3.3.5) is examined by first replacing

$u_{i,j}$ by $u_{m,n}$ and then letting $u_{m,n} = e^{im\gamma}\xi^n$, where γ is an

arbitrary real number and $\xi = e^{i\lambda}$, λ being a complex parameter.

Equation (3.3.5) thus becomes

$$(1-\beta_1\theta)e^{i(m-1)\gamma}\xi^{n+1} + 4(1+\beta_2\theta)e^{im\gamma}\xi^{n+1} + (1-\beta_3\theta)e^{i(m+1)\gamma}\xi^{n+1}$$

$$=\{1+\beta_1(1-\theta)\}e^{i(m-1)\gamma}\xi^n + 4\{1-\beta_2(1-\theta)\}e^{im\gamma}\xi^n + \{1+\beta_3(1-\theta)\}e^{i(m+1)\gamma}\xi^n$$

Dividing by $e^{im\gamma}\xi^n \neq 0$ and rearranging gives

$$\xi = \frac{\{1+\beta_1(1-\theta)\}e^{-i\gamma} + 4\{1-\beta_2(1-\theta)\} + \{1+\beta_3(1-\theta)\}e^{i\gamma}}{(1-\beta_1\theta)e^{-i\gamma} + 4(1+\beta_2\theta) + (1-\beta_3\theta)e^{i\gamma}}$$

If we now replace β_1, β_2, β_3 by their full expressions and let

h and k tend to zero in such a way that r remains fixed we

obtain

$$\xi = \frac{\{1 + 6ar(1-\theta)\}(e^{-i\gamma}+e^{i\gamma}) + 4\{1 - 3ar(1-\theta)\}}{(1 - 6ar\theta)(e^{-i\gamma}+e^{i\gamma}) + 4(1+3ar\theta)} \qquad (3.3.11)$$

Since $\qquad 2\cos\gamma = e^{-i\gamma}+e^{i\gamma}$,

and $\qquad \cos\gamma = 1 - 2\sin^2\frac{\gamma}{2}$

it follows that, in view of the fact that ξ is purely real, the

stability condition on ξ is

$$-1 \leqslant \frac{3 - 2(1 + 6ar(1-\theta))\sin^2\frac{\gamma}{2}}{3 - 2(1 - 6ar\theta)\sin^2\frac{\gamma}{2}} \leqslant 1 \qquad (3.3.12)$$

Denoting the denominator in this expression by D, we see

that since $r > 0$, $a > 0$ and $\theta \geqslant 0$ then $D > 0$. Thus (3.3.12)

becomes

$$- 3 + 2(1-6ar\theta)\sin^2\frac{\gamma}{2} \leqslant 3 - 2(1+6ar(1-\theta))\sin^2\frac{\gamma}{2} \leqslant 3 - 2(1-6ar\theta)\sin^2\frac{\gamma}{2} .$$

$$(3.3.13)$$

From the right-hand inequality in (3.3.13) we have

$$-12ar\sin^2\frac{\gamma}{2} \leqslant 0 \qquad (3.3.14)$$

which is satisfied for all $r > 0$; thus the left-hand

inequality will yield the required stability criteria.

From the left-hand inequality we obtain the expression

$$12ar(1-2\theta)\sin^2\frac{\gamma}{2} \leqslant 6 - 4\sin^2\frac{\gamma}{2} . \qquad (3.3.15)$$

Thus, if $1-2\theta > 0$, we can rearrange (3.3.15) to give

$$r \leqslant \frac{3 - 2\operatorname{Sin}^2\frac{\gamma}{2}}{6a(1-2\theta)\operatorname{Sin}^2\frac{\gamma}{2}} \quad . \qquad (3.3.16)$$

Since $\operatorname{Sin}^2\frac{\gamma}{2} \in [0,1]$, then by choosing $\operatorname{Sin}^2\frac{\gamma}{2}$ to give the most

restricted condition on stability, we obtain

$$r \leqslant \frac{1}{6a(1-2\theta)} \quad . \qquad (3.3.17)$$

Alternatively, if $1-2\theta \leqslant 0$, rearrangement of (3.3.15) gives

$$r \geqslant \frac{3 - 2\operatorname{Sin}^2\frac{\gamma}{2}}{6a(1-2\theta)\operatorname{Sin}^2\frac{\gamma}{2}} \qquad (3.3.18)$$

and thus $r \geqslant \alpha$, where $\alpha < 0$. This implies that the scheme

(3.3.5) is unconditionally stable for $1-2\theta \leqslant 0$.

The scheme (3.3.5) therefore has the following condition

governing its stability

(a)   if $\theta \geqslant \frac{1}{2}$, it is unconditionally stable.

(b)   if $\theta < \frac{1}{2}$, it is stable provided that

$$r \leqslant \{6a(1-2\theta)\}^{-1} \quad . \qquad (3.3.19)$$

3.4   Variable Coefficients

As shown in section 3.2 spline techniques can be applied

to hyperbolic partial differential equations with variable

coefficients. In this section we require solutions to the

parabolic equation with variable coefficients

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left[a(x,t)\frac{\partial u}{\partial x}\right] + b(x,t)\frac{\partial u}{\partial x} + c(x,t)u \qquad (3.4.1)$$

where again $a(x,t) > 0$ at all points in the solution domain.

As in previous sections, if we replace the time derivative

in (3.4.1) by a finite difference approximation and the

space derivatives by a cubic spline we obtain at (ih,jk)

$$\frac{u_{i,j+1} - u_{i,j}}{k} = \theta a_{i,j+1} M_{i,j+1} + (1-\theta)a_{i,j} M_{i,j}$$

$$+ \theta(a'_{i,j+1} + b_{i,j+1})L_{i,j+1} + (1-\theta)(a'_{i,j} + b_{i,j})L_{i,j}$$

$$+ \theta c_{i,j+1} u_{i,j+1} + (1-\theta)c_{i,j} u_{i,j} \qquad (3.4.2)$$

$(i=0,1,\ldots,N$; $j=1,2,\ldots$; $Nh=1$; $\theta \geqslant 0)$.

To obtain the required scheme incorporating cubic splines

we perform the following operations:

(i)   multiply (3.1.7) by $a_{i,j}(1-\theta)$;

(ii)   multiply (3.1.9) by $\theta a_{i,j+1}$;

(iii)   multiply (3.1.14) by $(a'_{i,j}+b_{i,j})(1-\theta)$;

(iv)   multiply (3.1.16) by $\theta(a'_{i,j+1}+b_{i,j+1})$;

(v)   add the expressions obtained in (i)-(iv) together;

      this gives the following expression

$$a_{i,j}(1-\theta)\left(\frac{1}{6}M_{i-1,j}+\frac{2}{3}M_{i,j}+\frac{1}{6}M_{i+1,j}\right) + a_{i,j+1}\theta\left(\frac{1}{6}M_{i-1,j+1}+\frac{2}{3}M_{i,j+1}+\frac{1}{6}M_{i+1,j+1}\right)$$

$$+(a'_{i,j}+b_{i,j})(1-\theta)\left(\frac{1}{6}L_{i-1,j}+\frac{2}{3}L_{i,j}+\frac{1}{6}L_{i+1,j}\right)+(a'_{i,j+1}+b_{i,j+1})\theta\left(\frac{1}{6}L_{i-1,j+1}\right.$$

$$\left. + \frac{2}{3}L_{i,j+1}+\frac{1}{6}L_{i+1,j+1}\right)$$

$$= a_{i,j}(1-\theta)\left(\frac{u_{i-1,j}-2u_{i,j}+u_{i+1,j}}{h^2}\right) + a_{i,j+1}\theta\left(\frac{u_{i-1,j+1}-2u_{i,j+1}+u_{i+1,j+1}}{h^2}\right)$$

$$+(a'_{i,j}+b_{i,j})(1-\theta)\left(\frac{u_{i+1,j}-u_{i-1,j}}{2h}\right) + (a'_{i,j+1}+b_{i,j+1})\theta\left(\frac{u_{i+1,j+1}-u_{i-1,j+1}}{2h}\right)$$

$$(3.4.3)$$

(vi)　use (3.4.2) directly and with i replaced by

both (i-1) and (i+1) to eliminate the $M_{i,j}$ and

$L_{i,j}$ values in (3.4.3). In the case of constant

coefficients the required scheme results immediately.

In this case however, use must also be made of Taylor

Series expansions before the M's and L's can be

eliminated. For example, (3.4.2) with i replaced

by (i-1) can be written as

$$
\frac{u_{i-1,j+1} - u_{i-1,j}}{k} = \theta\left(a_{i,j+1} - ha'_{i,j+1} + \frac{h^2}{2!}a''_{i,j+1}\cdots\right)M_{i-1,j+1}
$$

$$
+(1-\theta)\left(a_{i,j} - ha'_{i,j} + \frac{h^2}{2!}a''_{i,j}\cdots\right)M_{i-1,j}
$$

$$
+\theta\left(a'_{i,j+1} - ha''_{i,j+1}+\cdots+b_{i,j+1} - hb'_{i,j+1} + \frac{h^2}{2!}b''_{i,j+1}\cdots\right)
$$

$$
L_{i-1,j+1}
$$

$$
+(1-\theta)\left(a'_{i,j} - ha''_{i,j}+\cdots+b_{i,j} - hb'_{i,j} + \frac{h^2}{2!}b''_{i,j}\cdots\right)
$$

$$
L_{i-1,j}
$$

$$
+ \theta c_{i-1,j+1}\, u_{i-1,j+1} + (1-\theta)c_{i-1,j}\, u_{i-1,j} \qquad (3.4.4)
$$

A similar expression can also be obtained for (3.4.2)

with i replaced by (i+1). These expressions are then used

to carry out the elimination of the $M_{i,j}$ and $L_{i,j}$ values as

required. The following scheme thus results

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$$(\phi_{i-1,j+1} - \phi\psi_{i,j+1}) + 4(\phi_{i,j+1} + 3\theta\gamma_{i,j+1})u_{i,j+1}$$

$$+ (\phi_{i+1,j+1} - \theta\chi_{i,j+1})u_{i+1,j+1}$$

$$=\{\phi_{i-1,j} + kc_{i-1,j} + (1-\theta)\psi_{i,j}\}u_{i-1,j} + 4\{\phi_{i,j} + kc_{i,j} - 3(1-\theta)\gamma_{i,j}\}\ u_{i,j}$$

$$+\{\phi_{i+1,j} + kc_{i+1,j} + (1-\theta)\chi_{i,j}\}\ u_{i+1,j}$$

$$(i=1,2,\ldots,(N-1)) \qquad\qquad (3.4.5)$$

where

$$\phi_{i,j} = 1 - k\theta c_{i,j} \quad,\quad \gamma_{i,j} = ra_{i,j} \quad,\quad \psi_{i,j} = 6\gamma_{i,j} - \beta_{i,j} \quad,$$

$$\chi_{i,j} = 6\gamma_{i,j} + \beta_{i,j} \quad,\quad \beta_{i,j} = 3\frac{k}{h}(a'_{i,j} + b_{i,j}).$$

As in section 3.2, the stability condition for the scheme

(3.4.5) is derived by applying the von Neumann Method locally.

It can thus be shown that

(i)   if $\theta \geqslant \frac{1}{2}$, it is unconditionally stable

(ii)   if $\theta < \frac{1}{2}$, it is stable provided

$$r \leqslant \{\ 6a(x,t)(1-2\theta)\}^{-1} \qquad\qquad (3.4.6)$$

is satisfied independently at each point of the solution

domain.

The truncation error associated with (3.4.5) may again be

derived by expanding the terms in the scheme using Taylor

series. As in section 3.2, the expression is complicated

by derivatives of the variable coefficients. For conciseness

the details are not given here, but it can be shown that the

error of (3.4.5) is $O(k^2)$.

CHAPTER 4

Initial Value Partial Differential
Equations with Unequally Spaced Knots.

4.1   The Use of Unequal Step Lengths

The numerical solution of partial differential equations using

finite difference schemes in which the mesh points are non-

uniformly distributed has been considered by various authors.

For example, Saul'yev (1964) suggested the use of non-rectangular

grids for solving the heat conduction equation in which the

initial condition g(x) has the form illustrated in Figure 1.

Saul'yev recommends that, due to the changing nature of the

function g(x) in such a situation the step lengths should be

chosen to be smaller in the first third of the range $[0,1]$

and larger in the reamining two-thirds.

More complicated problems in which the solution varies rapidly

over a small part of the domain but very slowly over the rest

are found in boundary layer problems in fluid dynamics. Crowder

and Dalton (1971) and Kàlnay de Rivas (1972) have considered

the use of non-uniform grids which can be used to place sufficient

mesh points in the region of the boundary layer and fewer

points in the remaining solution domain.

Finite difference approximations with unequally spaced mesh

points have also been shown to be advantageous in moving

boundary problems in heat flow (see for example Murray and

Landis (1959), Douglas and Gallie (1955), Lotkin (1960)
and Crank and Gupta (1972a).

4.2 <u>Hyperbolic Partial Differential Equations with Constant Coefficients</u>

In this section we obtain solutions $u(x,t)$ to (3.1.1)

using spline techniques in which the knot partition (3.1.4)

is considered to be unequally spaced and where the distance

between successive knots is given in (2.2.2).

From equation (2.2.3) the spline function on the jth time

line has the form

$$S_j(x) = M_{i-1,j} \frac{(x_i - x)^3}{6h_i} + M_{i,j} \frac{(x - x_{i-1})^3}{6h_i} + \left(u_{i-1,j} - \frac{h_i^2 M_{i-1,j}}{6} \right) \frac{(x_i - x)}{h_i}$$

$$+ \left(u_{i,j} - \frac{h_i^2 M_{i,j}}{6} \right) \frac{(x - x_{i-1})}{h_i} \quad . \quad (i=1,2,\ldots,N) \qquad (4.2.1)$$

Similarly the expression (2.2.6) for the second derivative

of the spline function becomes on the jth time level

$$\frac{h_i M_{i-1,j}}{6} + \frac{h_i + h_{i+1}}{3} M_{i,j} + \frac{h_{i+1} M_{i+1,j}}{6}$$

$$= \frac{h_i u_{i+1,j} - (h_i + h_{i+1}) u_{i,j} + h_{i+1} u_{i-1,j}}{h_i h_{i+1}} \qquad (4.2.2)$$

$$(i=1,2,\ldots,(N-1))$$

A relationship similar to (3.1.14) is now required for unequally

spaced knots. From (3.1.10) to (3.1.13) the following expressions

are obtained

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$$h_i L_{i,j} = \frac{h_i^2}{6} M_{i-1,j} + \frac{h_i^2}{3} M_{i,j} + u_{i,j} - u_{i-1,j} \qquad (4.2.3)$$

$$h_{i+1} L_{i,j} = -\frac{h_{i+1}^2}{3} M_{i,j} - \frac{h_{i+1}^2}{6} M_{i+1,j} + u_{i+1,j} - u_{i,j} \qquad (4.2.4)$$

$$h_{i+1} L_{i+1,j} = \frac{h_{i+1}^2}{6} M_{i,j} + \frac{h_{i+1}^2}{3} M_{i+1,j} + u_{i+1,j} - u_{i,j} \qquad (4.2.5)$$

$$h_i L_{i-1,j} = -\frac{h_i^2}{3} M_{i-1,j} - \frac{h_i^2}{6} M_{i,j} + u_{i,j} - u_{i-1,j} \qquad (4.2.6)$$

Adding (4.2.3) and (4.2.4) to half the sum of (4.2.5) and

(4.2.6) gives the expression

$$\frac{h_i}{6} L_{i-1,j} + \frac{h_i + h_{i+1}}{3} L_{i,j} + \frac{h_{i+1}}{6} L_{i+1,j}$$

$$= \frac{(h_i^2 - h_{i+1}^2)}{12} M_{i,j} + \frac{u_{i+1,j} - u_{i-1,j}}{2} \qquad (4.2.7)$$

$$(i=1,2,\ldots,(N-1))$$

Approximations similar to (4.2.2) and (4.2.7) also hold on the

$(j-1)^{th}$ and $(j+1)^{th}$ time lines. As explained in section 3.1

we now take combinations of the above mentioned relationships

and use (3.1.5) to eliminate the $M_{i,j}$ and $L_{i,j}$ terms where

possible. The following three time level scheme is thus obtained

$$(\phi_i - \gamma_i \theta)u_{i-1,j+1} + 2(1 + \chi_i \theta)u_{i,j+1} + (\beta_i - \psi_i \theta)u_{i+1,j+1}$$

$$+ \frac{bk^2}{2}(h_{i+1} - h_i)(\theta M_{i,j-1} + (1-2\theta)M_{i,j} + \theta M_{i,j+1})$$

$$=\{2\phi_i + \gamma_i(1-2\theta)\}u_{i-1,j} + 2\{2 - \chi_i(1-2\theta)\}u_{i,j} + \{2\beta_i + \psi_i(1-2\theta)\}u_{i+1,j}$$

$$-(\phi_i - \gamma_i \theta)u_{i-1,j-1} - 2(1 + \chi_i \theta)u_{i,j-1} - (\beta_i - \psi_i \theta)u_{i+1,j-1} \qquad (4.2.8)$$

$$(i=1,2,\ldots,(N-1))$$

where

$$\gamma_i = 6ar_i - 3bh_{i+1}s_i + ch_i h_{i+1}s_i$$

$$\chi_i = 6a\nu_i - ck^2$$

$$\psi_i = 6as_i + 3bh_i r_i + ch_i h_{i+1}r_i$$

$$\phi_i = \frac{h_i}{h_i + h_{i+1}} \quad , \quad \beta_i = \frac{h_{i+1}}{h_i + h_{i+1}}$$

and the mesh ratios r_i, s_i and ν_i are given by

$$r_i = \frac{k^2}{h_i(h_i + h_{i+1})} \quad , \quad s_i = \frac{k^2}{h_{i+1}(h_i + h_{i+1})} \quad , \quad \nu_i = \frac{k^2}{2h_i h_{i+1}} \quad .$$

If the coefficient b in (3.1.1) is non-zero the solution

of the scheme (4.2.8) is complicated by the presence of

$M_{i,j-1}$, $M_{i,j}$ and $M_{i,j+1}$. Assuming that the scheme is fully

developed in that values for u and M are known on the jth

and $(j-1)^{th}$ time lines, then we must determine $M_{i,j+1}$ values

before further solutions $u_{i,j+1}$ can be found.

This problem is overcome using the following numerical

procedure:

(i)   Using the initial condition (3.1.3) the expression

     (4.2.2) becomes

$$\frac{h_i}{6}M_{i-1,0} + \frac{h_i + h_{i+1}}{3}M_{i,0} + \frac{h_{i+1}}{6}M_{i+1,0}$$

$$= \frac{h_i\, g_1(x_{i+1}) - (h_i + h_{i+1})g_1(x_i) + h_{i+1}g_1(x_{i-1})}{h_i h_{i+1}} \quad (4.2.9)$$

$$(i=1,2,\ldots,(N-1)$$

Given that $M_{0,j} = M_{N,j} = 0$ $(j=0,1,2,\ldots)$, the tri-diagonal

system is easily solved for $M_{i,0}$ $(i=1,2,\ldots,(N-1))$.

(ii)   By setting $\theta=0$ and using the derivative initial

     condition in (3.1.3), the scheme (4.2.8) becomes,

     with $j=0$

$$2\phi_i\, u_{i-1,1} + 4u_{i,1} + 2\beta_i\, u_{i+1,1} + \frac{bk^2}{2}(h_{i+1} - h_i)M_{i,0}$$

$$= (2\phi_i + \gamma_i)g_1(x_{i-1}) + 2(2-\chi_i)g_1(x_i) + (2\beta_i + \psi_i)g_1(x_{i+1})$$

$$+ 2k\phi_i g_2(x_{i-1}) + 4kg_2(x_i) + 2k\beta_i g_2(x_{i+1}). \quad (4.2.10)$$

$$(i=1,2,\ldots,(N-1))$$

The solutions $u_{i,1}(i=1,2,\ldots,(N-1))$ are thus obtained from

tri-diagonal system (4.2.10).

(iii)   Putting j=1 in the expression (4.2.2) gives an easily

solvable tri-diagonal system of equations producing

the values $M_{i,1}$ (i=1,2,.....,(N-1)).

(iv)   Since we have now determined $M_{i,0}$, $M_{i,1}$, $u_{i,0}$ and

$u_{i,1}$ we can develop a general scheme for obtaining

$M_{i,j+1}$ and hence $u_{i,j+1}$. This is done using a simple

iterative process, beginning with an initial approximation

$M_{i,j+1}^{(0)}$ to $M_{i,j+1}$, given by the extrapolated relationship

$$M_{i,j+1}^{(0)} = 2M_{i,j} - M_{i,j-1} \quad (i=0,1,.....,N). \qquad (4.2.11)$$

We substitute (4.2.11) into the scheme (4.2.8) thus

obtaining initial approximations $u_{i,j+1}^{(0)}$, to $u_{i,j+1}$.

(v)   Assuming now that the iterative process is fully

developed and that we wish to obtain improved

approximations $M_{i,j+1}^{(n+1)}$, to $M_{i,j+1}$, then from (4.2.2)

we have the expression

$$\frac{h_i M_{i-1,j+1}^{(n+1)}}{6} + \frac{h_i + h_{i+1}}{3} M_{i,j+1}^{(n+1)} + \frac{h_{i+1}}{6} M_{i+1,j+1}^{(n+1)}$$

$$= \frac{h_i u_{i+1,j+1}^{(n)} - (h_i + h_{i+1}) u_{i,j+1}^{(n)} + h_{i+1} u_{i-1,j+1}^{(n)}}{h_i h_{i+1}} \cdot (4.2.12)$$

Given that $M_{0,j+1}^{(n+1)} = M_{N,j+1}^{(n+1)} = 0$, the system (4.2.12)

is easily solved for the required improved approximations

$M_{i,j+1}^{(n+1)}$ (i=1,2,.....,(N-1)).

(vi)   The $M_{i,j+1}^{(n+1)}$ values obtained in (v) are now used in the scheme (4.2.8), which in iterative notation is

$$(\phi_i - \gamma_i\theta)u_{i-1,j+1}^{(n+1)} + 2(1+\chi_i\theta)u_{i,j+1}^{(n+1)} + (\beta_i - \psi_i\theta)u_{i+1,j+1}^{(n+1)}$$

$$+ \frac{bk^2}{2}(h_{i+1} - h_i)(\theta M_{i,j-1} + (1-2\theta)M_{i,j} + \theta M_{i,j+1}^{(n+1)})$$

$$= \{2\phi_i + \gamma_i(1-2\theta)\}u_{i-1,j} + 2\{2-\chi_i(1-2\theta)\}u_{i,j} + \{2\beta_i + \psi_i(1-2\theta)\}u_{i+1,j}$$

$$-(\phi_i-\gamma_i\theta)u_{i-1,j-1} - 2(1+\chi_i\theta)u_{i,j-1} - (\beta_i-\psi_i\theta)u_{i+1,j-1}$$

$$(i=1,2,\ldots,(N-1)) \qquad (4.2.13)$$

By solving (4.2.13) we obtain improved approximations $u_{i,j+1}^{(n+1)}$, to $u_{i,j+1}$.

(vii)   A test is now performed on these $u_{i,j+1}^{(n+1)}$ values by examining numerical values of the inequality

$$\left| u_{i,j+1}^{(n+1)} - u_{i,j+1}^{(n)} \right| \leqslant \epsilon \qquad (i=1,2,\ldots,(N-1)) \quad (4.2.14)$$

for some fixed tolerance ϵ. If (4.2.14) is satisfied for all i then the $u_{i,j+1}^{(n+1)}$ are taken as the required solutions. However, if (4.2.14) is not satisfied, then the $u_{i,j+1}^{(n+1)}$ must be re-employed in (4.2.12) and the process repeated until the required accuracy is achieved.

The obtaining of solutions to (3.1.1) using this iterative process is obviously more computationally expensive than the previously described equally spaced knot schemes. However,

the M values obtained in this process are of further

benefit in the following instances:

(a)   As explained in Wisher (1977), a major advantage
       over finite difference approximations
       of splines schemes is that by making use of the
                         ₕ
       spline function (4.1.1), we can easily obtain

       solutions to (3.1.1) at points intermediate to

       the knot points.

(b)   In a later section of this thesis an algorithm is

       derived for obtaining 'optimal' knot positions for

       the spline solution of partial differential equations.

       This algorithm requires the evaluation of the $M_{i,j}$

       values on each time line.

The truncation error for the scheme (4.2.8) may again be

derived using Taylor Series expansions. For example,

expanding $u_{i+1,j}$ and $u_{i-1,j}$ about (x_i, t_j) we have

$$u_{i+1,j} = u_{i,j} + h_{i+1}\left(\frac{\partial u}{\partial x}\right)_{i,j} + \frac{h_{i+1}^2}{2!}\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} + \dots \qquad (4.2.15)$$

and

$$u_{i-1,j} = u_{i,j} - h_i\left(\frac{\partial u}{\partial x}\right)_{i,j} + \frac{h_i^2}{2!}\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} - \dots \qquad (4.2.16)$$

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The following expression for the truncation error is thus obtained

$$k^2 \left[c^2 k^2 f(\theta) u + \left\{ 2bck^2 f(\theta) + \frac{1}{3} c^2 k^2 \theta (h_i - h_{i+1}) \right\} \frac{\partial u}{\partial x} \right.$$

$$+ \left\{ k^2 (2ac+b^2) f(\theta) + \frac{1}{6} b(h_i - h_{i+1})(1+ck^2\theta) - \frac{1}{3} c^2 k^2 \theta \left(\frac{h_i^3 + h_{i+1}^3}{h_i + h_{i+1}} \right) \right\} \frac{\partial^2 u}{\partial x^2}$$

$$+ \left\{ 2abk^2 f(\theta) + \frac{1}{6} k^2 \theta (h_i - h_{i+1})(2ac+3b^2) - \frac{1}{18} c \left(\frac{h_i^4 - h_{i+1}^4}{h_i + h_{i+1}} \right) \right.$$

$$\left. - \frac{1}{6} bck^2 \theta \left(\frac{h_i^3 + h_{i+1}^3}{h_i + h_{i+1}} \right) \right\} \frac{\partial^3 u}{\partial x^3}$$

$$+ \left\{ a^2 k^2 f(\theta) + \frac{1}{2} abk^2 \theta (h_i - h_{i+1}) + \frac{1}{12} a \left(\frac{h_i^3 + h_{i+1}^3}{h_i + h_{i+1}} \right) (1-2ck^2\theta) \right.$$

$$\left. \left. + \frac{1}{24} b \left(\frac{h_i^4 - h_{i+1}^4}{h_i + h_{i+1}} \right) - \frac{1}{72} c \left(\frac{h_i^5 + h_{i+1}^5}{h_i + h_{i+1}} \right) \right\} \frac{\partial^4 u}{\partial x^4} \right] \qquad (4.2.17)$$

where $f(\theta)$ is given by (3.1.19)

Due to the unequally spaced knot points employed in the scheme (4.2.8) it is not possible to examine the stability of this scheme using the usual von Neumann method. This is because the method requires that the step lengths h and k tend to zero in such a way that the mesh ratio r remains fixed. In (4.2.8) each mesh ratio involves both h_i and h_{i+1},

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which we would have to let tend to zero at the same rate.
However, the scheme (4.2.8) reduces to (3.1.17) when
$h_i = h_{i+1} = h$ and we would thus expect the stability
conditions for the two schemes to be very similar.

This problem has been considered by Saul'yev (1964) in the
use of non-uniform finite difference approximations. Using
his notation the reasoning of the above paragraph suggests
that the scheme (4.2.8) has the following stability condition

(a)   if $\theta \geqslant \frac{1}{4}$, it is unconditionally stable

(b)   if $\theta < \frac{1}{4}$, it is stable provided that

$$\frac{k^2}{\min\{h_i h_{i+1}\}} \leqslant \frac{1}{3a(1-4\theta)} \tag{4.2.18}$$

Numerical evidence confirming this stability condition is
given in the later chapters on case studies where values
of θ, k, h_i and h_{i+1} are used which either satisfy or
violate the condition.

4.3   Parabolic Partial Differential Equations with
       Constant Coefficients

Here we consider spline solutions to the parabolic equation
(3.3.1). As in the previous section the knot partition (3.1.4)
is chosen to be unequally spaced where h_i, the distance
between successive knots, is given by (2.2.2).

Using the technique explained in section 3.3, we take

combinations of the relationships (4.2.2) and (4.2.7) and use

(3.3.4) to eliminate the $M_{i,j}$ and $L_{i,j}$ terms where possible.
The two time level scheme thus obtained is as follows

$$(\phi_i - \gamma_i\theta)u_{i-1,j+1} + 2(1 + \chi_i\theta)u_{i,j+1} + (\beta_i - \psi_i\theta)u_{i+1,j+1}$$

$$+ \frac{bk(h_{i+1} - h_i)}{2}(\theta M_{i,j+1} + (1-\theta)M_{i,j})$$

$$=\{\phi_i + \gamma_i(1-\theta)\}u_{i-1,j} +2\{1-\chi_i(1-\theta)\}u_{i,j} +\{\beta_i+\psi_i(1-\theta)\}u_{i+1,j}$$

$$(i=1,2,\ldots,(N-1)) \qquad (4.3.1)$$

where $\gamma_i,\psi_i,$ ϕ_i and β_i are as defined in section 4.2 and

$$\chi_i = 6a\nu_i - ck,$$

$$r_i = \frac{k}{h_i(h_i + h_{i+1})} \quad , \quad s_i = \frac{k}{h_{i+1}(h_i+h_{i+1})} \quad , \quad \nu_i \quad \frac{k}{2h_i h_{i+1}} \quad .$$

As described in section 4.2, when the coefficient b in (3.3.1)

is non-zero the scheme (4.3.1) requires the calculation of

$M_{i,j+1}$ and $M_{i,j}$ before solutions can be produced. A numerical

procedure similar to that of the previous section is employed,

although in this case the process is considerably simplified

since (4.3.1) is only a two time level scheme. The numerical

procedure is briefly as follows:

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(i)   Using the expression (4.2.2) determine $M_{i,0}(i=1,2,....,(N-1))$.

(ii)   Set $\theta = 0$ in (4.3.1) and hence evaluate the solutions

        $u_{i,1}(i=1,2,....,(N-1))$.

(iii)   Using (4.2.2) determine $M_{i,1}(i=1,2,...,(N-1))$.

(iv)   Evaluate $u_{i,2}(i=1,2,...,(N-1))$ from the scheme

        (4.3.1).

The procedure is now fully developed and further solutions

are obtained using (4.2.2) and (4.3.1) alternately.

In a similar manner to previous sections, we again derive the

truncation error associated with the scheme (4.3.1) using

Taylor series expansions. It can thus be shown that (4.3.1)

becomes

$$\left[-\gamma_i+2\chi_i-\psi_i\right] u + \left[k(3-\gamma_i\theta+2\chi_i\theta-\psi_i\theta)\right]\frac{\partial u}{\partial t}$$

$$+ \left[\frac{k^2}{2}(3-\gamma_i\theta+2\chi_i\theta-\psi_i\theta)\right]\frac{\partial u^2}{\partial t^2} + \left[\frac{k^3}{6}(3-\gamma_i\theta+2\chi_i\theta-\psi_i\theta)\right]\frac{\partial^3 u}{\partial t^3}$$

$$+ \left[\frac{k^4}{24}(3-\gamma_i\theta+2\chi_i\theta-\psi_i\theta)\right]\frac{\partial^4 u}{\partial t^4} + \left[h_i\gamma_i - h_{i+1}\psi_i\right]\frac{\partial u}{\partial x}$$

$$+ \left[-k(h_i - h_{i+1})+ k(h_i\gamma_i\theta - h_{i+1}\psi_i\theta)\right]\frac{\partial^2 u}{\partial x\partial t}$$

$$+ \left[-\frac{k^2}{2}(h_i - h_{i+1})+ \frac{k^2}{2}(h_i\gamma_i\theta - h_{i+1}\psi_i\theta)\right]\frac{\partial^3 u}{\partial x\partial t^2}$$

$$+ \left[-\frac{k^3}{6}(h_i-h_{i+1})+ \frac{k^3}{6}(h_i\gamma_i\theta-h_{i+1}\psi_i\theta)\right]\frac{\partial^4 u}{\partial x\partial t^3} + \left[-\frac{h_i^2}{2}\gamma_i-\frac{h_{i+1}^2}{2}\psi_i\right]\frac{\partial^2 u}{\partial x^2}$$

$$+ \left[\frac{k}{2}(h_i^2(\phi_i-\gamma_i\theta)+h_{i+1}^2(\beta_i-\psi_i\theta))\right]\frac{\partial^3 u}{\partial x^2\partial t}$$

$$+ \left[\frac{k^2}{4}(h_i^2(\phi_i-\gamma_i\theta)+h_{i+1}^2(\beta_i-\psi_i\theta))\right]\frac{\partial^4 u}{\partial x^2\partial t^2} + \left[\frac{h_i^3}{6}\gamma_i - \frac{h_{i+1}^3}{6}\psi_i\right]\frac{\partial^3 u}{\partial x^3}$$

$$+ \left[-\frac{k}{6}(h_i^3(\phi_i-\gamma_i\theta)-h_{i+1}^3(\beta_i-\psi_i\theta))\right]\frac{\partial^4 u}{\partial x^3\partial t} + \left[-\frac{h_i^4}{24}\gamma_i - \frac{h_{i+1}^4}{24}\psi_i\right]\frac{\partial^4 u}{\partial x^4}$$

                                                         (4.3.2)

This expression again contains time and mixed

derivative terms. As in section 3.3, these can be replaced

using (3.3.1), although the resulting expression is

extremely complicated due to the variable step lengths.

In the simple case of the heat conduction equation ((3.3.1) with

a=1, b=c=0) the truncation error to fourth order derivative

terms has the form

$$
k \left[\frac{k}{2} + \frac{1}{12} \left(\frac{h_i^3 + h_{i+1}^3}{h_i + h_{i+1}} \right) - k\theta \right] \frac{\partial^4 u}{\partial x^4} + \dots \qquad (4.3.3)
$$

In addition, the scheme (4.3.1) has the following conditions

governing its stability

(a)   if $\theta \geqslant \frac{1}{2}$, it is unconditionally stable

(b)   if $\theta < \frac{1}{2}$, it is stable provided that

$$
\frac{k}{\min\{h_i h_{i+1}\}} \quad \leqslant \quad \frac{1}{6a(1-2\theta)} \qquad \qquad (4.3.4)
$$

CHAPTER 5

Methods for Obtaining Knot Partitions

5.1   Preamble

In this chapter three techniques are presented for

obtaining 'optimal' knot partitions. These techniques

will be called the 'local', 'global' and 'transformation' methods

for reasons which will become apparent. The knot partitions

obtained are chosen to best suit (in some sense) the initial

condition of the partial differential equation, but which

are then fixed throughout time.

As explained in the work of de Boor (1978), we cannot hope

to place each knot optimally. This is because in approximating

a function $f(x)$ by a spline function $S(x)$ we must have

sufficient information about $f(x)$ to evaluate $||f-S||_\infty$

before each knot can be optimally located. In the solution

of differential equations $f(x)$ is only known implicitly

and hence in this thesis we endeavour to obtain an optimum

knot distribution which we believe to be a general improvement

on existing equally spaced knot methods. More exactly one could

consider the knots as sub-optimal. Here-after the word optimal

will have this meaning.

5.2   A Local Method

The technique described in this section for obtaining

optimal knot positions is an adaptation of the well-known

work of Curtis and Powell (1967). In that work, the authors

developed an algorithm for use in approximating simple

functions using cubic splines. They stated than an estimate

ε_i of the error $\varepsilon(x) = f(x) - S(x)$ at each knot x_i is given by

$$\varepsilon_i = ||f - S||_\infty \simeq \frac{1}{384} (x_i - x_{i-1})^3 d_i \qquad (5.2.1)$$

where d_i, the discontinuity in the third derivative of the

spline function, is defined as

$$d_i = S'''(x_i+) - S'''(x_i-). \qquad (5.2.2)$$

A full derivation of (5.2.1) is given in Schultz (1973).

We now require an expression for this discontinuity in

terms of function values $f(x)$.

Rewriting (3.1.7) we have

$$S''(x_{i-1}) + 4S''(x_i) + S''(x_{i+1}) = \frac{6}{h^2}\left[f(x_{i-1}) - 2f(x_i) + f(x_{i+1})\right] \quad (5.2.3)$$

which in operator notation can be written as

$$(E^{-1} + 4 + E)h^2 S''(x_i) = 6(E^{-1} - 2 + E)f(x_i) \qquad (5.2.4)$$

and after rearrangement

$$h^2 S''(x_i) = \frac{6(E^{-1} - 2 + E)}{E^{-1} + 4 + E} f(x_i). \qquad (5.2.5)$$

Using a simple forward difference approximation, $S'''(x_i+)$ can be expressed as

$$S'''(x_i+) = \frac{S''(x_{i+1}) - S''(x_i)}{h} \qquad (5.2.6)$$

and thus by substituting for the second derivatives using (5.2.5), we have the expression

$$h^3 S'''(x_i+) = \frac{6(E^{-1}-2+E)}{E^{-1}+4+E} f(x_{i+1}) - \frac{6(E^{-1}-2+E)}{E^{-1}+4+E} f(x_i) . \qquad (5.2.7)$$

Employing the shift operator again, (5.2.7) becomes

$$h^3 S'''(x_i+) = \frac{6(1-2E+E^2)}{E^{-1}+4+E} f(x_i) - \frac{6(E^{-1}-2+E)}{E^{-1}+4+E} f(x_i) . \qquad (5.2.8)$$

and thus after suitable rearrangement the following expression for $S'''(x_i+)$ is derived

$$h^3 S'''(x_i+) = \frac{6(3-3E+E^2-E^{-1})}{E^{-1}+4+E} f(x_i). \qquad (5.2.9)$$

Similarly, using the approximation

$$S'''(x_i-) = \frac{S''(x_i) - S''(x_{i-1})}{h} \qquad (5.2.10)$$

an expression for $S'''(x_i-)$ becomes

$$h^3 S'''(x_i-) = \frac{6(3E^{-1} - 3 + E - E^{-2})}{E^{-1} + 4 + E} f(x_i) . \qquad (5.2.11)$$

Subtracting the relationships (5.2.11) from (5.2.9)

results in the expression

$$S'''(x_i+) - S'''(x_i-) = \frac{6(6 - 4E + E^2 - 4E^{-1} + E^{-2})}{E^{-1} + 4 + E} f(x_i) \quad (5.2.12)$$

and thus

$$S'''(x_i+) - S'''(x_i-) \underset{\sim}{\sim} \frac{6hf^{iv}(x_i)}{E^{-1} + 4 + E}. \quad (5.2.13)$$

By expanding the denominator terms in (5.2.13) we obtain

approximately

$$S'''(x_i+) - S'''(x_i-) = h\left[1 + \frac{h^2D^2}{6} + \frac{h^4D^4}{72} + \ldots\right]^{-1} f^{iv}(x_i). \quad (5.2.14)$$

and hence, by ignoring $O(h^4)$ terms, (5.2.14) results in the

required expression for d_i

$$d_i = S'''(x_i+) - S'''(x_i-) = hf^{iv}(x_i) + O(h^3). \quad (5.2.15)$$

Employing Taylor's theorem to remove the higher order

terms in (5.2.15), the error estimate (5.2.1) thus becomes

$$\varepsilon_i = \frac{1}{384} h^4 f^{iv}(\xi) \quad (5.2.16)$$

where ξ is some value lying between x_{i-1} and x_i.

In the Curtis and Powell algorithm a cubic spline is

fitted to the function $f(x)$ using a small number of

equally spaced knots and if ε_i exceeds some pre-assigned

error bound, extra knots are inserted half-way between

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existing knots. The process is repeated until the

error estimates $|\varepsilon_i|$ are all less than the error bound.

To obtain unequal knot positions for use in the spline

solution of partial differential equations we rewrite

the error estimate (5.2.16) in the form

$$|\varepsilon_i| = |S_i - u_i| = \frac{1}{384} h_i^4 |u^{iv}(\xi)| \qquad (5.2.17)$$

where S_i and u_i are, respectively, the spline and exact

solutions at the knot x_i. Rearrangement of (5.2.17) yields

the expression

$$h_i = \left[\frac{384 \, \varepsilon_i}{|u^{iv}(\xi)|} \right]^{1/4} . \qquad (5.2.18)$$

Substitution of (5.2.18) into (2.2.2) gives the approximation

$$x_i = x_{i-1} + \left[\frac{384 \, \varepsilon_i}{|u^{iv}(\xi)|} \right]^{1/4} \qquad (i=1,2,\ldots,N) \qquad (5.2.19)$$

which may be used as a basis for generating suitable knot

partitions, in which the function $u^{iv}(\xi)$ is evaluated as the

fourth derivative of the initial condition at the knot x_{i-1}.

As will be later shown, equation (5.2.19) is implemented

with $\varepsilon = \varepsilon_1 = \varepsilon_2 = \ldots. = \varepsilon_N$, the aim being to choose a

suitable ε value which gives a desired number of knots

over $[0,1]$. This is only to enable us to compare the various

methods and in practice a bound would initially be
fixed on ε_i. The number and position of knots would
then be determined by this bound.

5.3   A Global Method

Here the technique described for obtaining knot partitions
for use in the spline solution of partial differential
equations is largely based on the work of de Boor (1973 and
1974). Using results obtained by Rice (1969), Phillips (1970),
McClure (1970), Dobson (1972), de Boor and Swartz (1973) and
Burchard (1974), de Boor considered the approximation of a
given function f on $\left[a,b\right]$ by S_Δ^k , a spline of order k
(degree k-1) with a knot partition Δ, where

$$\Delta: \quad a = t_1 < t_2 < \ldots < t_N < t_{N+1} = b. \tag{5.3.1}$$

For convenience only, (5.3.1) is here used rather than
(2.1.1); note that the notations are made compatible at the
end of this section.

To obtain suitable knot distributions, de Boor suggests
that the following condition should be satisfied

$$||f - S_\Delta||_i \leqslant C|\Delta t_i|^k \, ||f^{(k)}||_i + O(|\Delta|^k) \tag{5.3.2}$$

where

$$||h||_i \approx \sup_{t\varepsilon\left[t_i, t_{i+1}\right]} |h(t)| \quad , \tag{5.3.3}$$

$$|\Delta| = \max_i \Delta t_i = \max_i (t_{i+1} - t_i) \tag{5.3.4}$$

and C is a constant > 0. The norm $||f^{(k)}||_i$ can be illustrated pictorially as in Figure 2(a), and for sufficiently small $|\Delta|$ the expression (5.3.2) has the form shown in Figure 2(b).

Generalising (5.3.2) to the whole partition $\left[t_1, t_{N+1}\right]$ we obtain the condition

$$||f - S_\Delta||_\infty \leqslant \max_i ||f - S_\Delta||_i \approx C \max_i |\Delta t_i|^k ||f^{(k)}||_i \qquad (5.3.5)$$

which again is illustrated in Figure 3. This suggests that the knots $t_2, t_3, \ldots, t_N$ should be chosen such that

$$\max_i ||f - S_\Delta||_i \qquad (5.3.6)$$

is minimised. Since C is constant we thus require to minimise

$$\max_i \left[|\Delta t_i|^k \sup_{\left[t_i, t_{i+1}\right]} |f^{(k)}| \right] \qquad (5.3.7)$$

$$= \max_i \left[|t_{i+1} - t_i|^k \sup_{\left[t_i, t_{i+1}\right]} |f^{(k)}| \right]. \qquad (5.3.8)$$

Consider now a particular interval $\left[\alpha, \beta\right]$ and define the function $s(\alpha, \beta)$ to be

$$s(\alpha, \beta) = (\beta - \alpha)^k \sup_{\left[\alpha, \beta\right]} |f^{(k)}|. \qquad (5.3.9)$$

Fixing α and letting $\beta = \beta_1$ (say) we have from (5.3.9)

$$s(\alpha,\beta_1) = (\beta_1 - \alpha)^k \sup_{\left[\alpha,\beta_1\right]} \left|f^{(k)}\right| . \qquad (5.3.10)$$

If we now increase β to $\beta_2 = \beta_1 + \delta\beta_i$ then

$$\sup_{\left[\alpha,\beta_2\right]} \left|f^{(k)}\right| \geqslant \sup_{\left[\alpha,\beta_1\right]} \left|f^{(k)}\right| \qquad (5.3.11)$$

since in the new interval $\left[\alpha,\beta_2\right]$ $\left|f^{(k)}\right|$ may achieve a new maximum or may not. In addition, since

$$(\beta_2 - \alpha)^k > (\beta_1 - \alpha)^k \qquad (5.3.12)$$

then

$$s(\alpha,\beta_2) > s(\alpha,\beta_1). \qquad (5.3.13)$$

Similarly, if β is decreased to $\beta_2 = \beta_1 - \delta\beta_1$ we have

$$\sup_{\left[\alpha,\beta_2\right]} \left|f^{(k)}\right| \leqslant \sup_{\left[\alpha,\beta_1\right]} \left|f^{(k)}\right| \qquad (5.3.14)$$

and since

$$(\beta_2 - \alpha)^k < (\beta_1 - \alpha)^k \qquad (5.3.15)$$

then

$$s(\alpha,\beta_2) < s(\alpha,\beta_1) . \qquad (5.3.16)$$

We can thus conclude that the function $s(\alpha,\beta)$ is monotone increasing in β with α fixed.

Consider now the case when β is fixed and $\alpha = \alpha_1$ (say).

The expression (5.3.9) then becomes

$$s(\alpha_1,\beta) = (\beta - \alpha_1)^k \sup_{[\alpha_1,\beta]} |f^{(k)}| . \qquad (5.3.17)$$

If α is increased to $\alpha_2 = \alpha_1 + \delta\alpha_1$ then

$$\sup_{[\alpha_2,\beta]} |f^{(k)}| \leqslant \sup_{[\alpha_1,\beta]} |f^{(k)}| \qquad (5.3.18)$$

and since

$$(\beta - \alpha_2)^k < (\beta - \alpha_1)^k \qquad (5.3.19)$$

we have

$$s(\alpha_2,\beta) < s(\alpha_1,\beta). \qquad (5.3.20)$$

Similarly, if α is decreased to $\alpha_2 = \alpha_1 - \delta\alpha_1$ then it can be shown that

$$s(\alpha_2,\beta) > s(\alpha_1,\beta) \qquad (5.3.21)$$

and thus the function $s(\alpha,\beta)$ is monotone decreasing in α with β fixed.

Let us now consider a single break point t_2, with adjacent knots t_1 and t_3 fixed, as shown diagrammatically in Figure 4(a). If, as illustrated,

$$s(t_1,t_2) > s(t_2,t_3) \qquad (5.3.22)$$

then by moving t_2 to $t_2' = t_2 - \delta t_2$, we have

$$s(t_1, t_2') < s(t_1, t_2) \qquad (5.3.23)$$

as shown in Figure 4(b). In addition

$$s(t_2', t_3) > s(t_2, t_3) \qquad (5.3.24)$$

and we thus find that

$$\left| s(t_1, t_2') - s(t_2', t_3) \right| < \left| s(t_1, t_2) - s(t_2, t_3) \right|. \qquad (5.3.25)$$

Therefore to minimise the deviation $\left| s(t_1, t_2) - s(t_2, t_3) \right|$ t_2' should be chosen such that

$$s(t_1, t_2') = s(t_2', t_3). \qquad (5.3.26)$$

Similarly, (5.3.26) holds if the condition (5.3.22) has the form

$$s(t_1, t_2) < s(t_2, t_3). \qquad (5.3.27)$$

Generalising the above to the whole knot partition Δ it can thus be shown that $t_2, t_3, \ldots, t_N$ should be chosen such that

$$s(t_i, t_{i+1}) = \text{constant} \qquad (i=1,2,\ldots,N) \qquad (5.3.28)$$

in which case (5.3.8) is minimised . The expression (5.3.28) can be rewritten as

$$\left| t_{i+1} - t_i \right| \left(\left| \left| f^{(k)} \right| \right|_\infty \right)^{1/k} = \text{constant} \qquad (5.3.29)$$

and thus the knots $t_2, t_3, \ldots, t_N$ should be chosen such that

$$\int_{t_i}^{t_{i+1}} |f^{(k)}(x)|^{1/k} \, dx = \frac{1}{N} \int_0^1 |f^{(k)}(x)|^{1/k} \, dx \, . \qquad (5.3.30)$$

$$(i=1,2,\ldots,N)$$

To employ this technique in deriving knot partitions for the spline solution of partial differential equations we again apply the strategy of section 5.2 and take the function $f(x)$ to be the given initial condition (denoted by $g(x)$ in chapter 3). Since in this thesis we use cubic splines with knots $x_0, x_1, \ldots, x_N$ as defined by (3.1.4), the integral expression (5.3.30) becomes

$$\int_{x_i}^{x_{i+1}} |g^{iv}(x)|^{1/4} \, dx = \frac{1}{N} \int_0^1 |g^{iv}(x)|^{1/4} dx \, . \qquad (5.3.31)$$

$$(i=0,1,\ldots,(N-1))$$

5.4   A Transformation Method

As shown by Kálnay de Rivas (1972) and Blottner (1975)
the determination of suitable mesh points for the finite
difference solution of boundary layer problems is available
using co-ordinate transformations. Their idea is to make
a change of independent variable, mapping the domain into
a new co-ordinate system where the variations of the
solution are less rapid. Assuming that the transformation
is defined by

$$x = X(\xi) \tag{5.4.1}$$

where x is the old independent variable and ξ the new
one, then to resolve the boundary layers, a transformation
is required which stretches the independent variable in areas
of rapid change and compresses it elsewhere (see Figure 5).
This technique has been applied to several practical problems
by Jones and Thompson (1980) who also suggest several possible
types of transformation. For example, to resolve a boundary
layer near x=0, the transformation

$$x(\xi) = \xi^2 \tag{5.4.2}$$

is suggested and alternatively for boundary layers at both
x=0, and x=1, the transformation

$$X(\xi) = \sin^2(\pi\xi/2) \tag{5.4.3}$$

is appropriate.

In all the above references, the authors choose the

mesh points ξ_i to be equally spaced and generate the

non-uniform grid points x_i from the transformation (5.4.1).

They then obtain the required solutions by using simple

equally spaced finite difference approximations on the

transformed differential equation. In the present work,

once the unequally spaced knot partition has been obtained

using (5.4.1), the solutions are obtained using the

schemes of chapter 4. This avoids any analytical differentiation

of the transformation function $X(\xi)$.

As in the two previous sections the choice of a suitable

transformation (5.4.1) here depends on the shape of the

initial condition of the partial differential equation.

Suppose, for example, that the initial condition $g(x)$

is a continuous function having one peak (for example,

as in figure 1) at some point $x=\alpha$. The required transformation

should be chosen so as to 'bunch' the knots around $x=\alpha$ which

can be achieved by choosing $x=\xi^{\frac{1}{2}}$ to the left of the peak and

$x=\xi^2$ to the right of the peak as illustrated in figure 6.

Considering the area to the right of $x=\alpha$, we require

$$ x \;=\; A(\xi-\alpha)^2 + \alpha \qquad\qquad (5.4.4) $$

to be satisfied for some constant A. Since we also require

$x=1$ when $\xi=1$, then

$$A = \frac{1}{1 - \alpha} \qquad\qquad (5.4.5)$$

and thus to the right of the peak the knots are chosen according to the relationship

$$x = \frac{1}{1 - \alpha} (\xi-\alpha)^2 + \alpha . \qquad\qquad (5.4.6)$$

Similarly, it can be shown that to the left of the peak the knots should be chosen from the expression

$$x = (\alpha\xi)^{\frac{1}{2}} \qquad\qquad (5.4.7)$$

Additionally, a knot is positioned at the peak $x=\alpha$.

Assuming, for example, that the initial condition has a peak at $x=0.8$, then the relationships (5.4.6) and (5.4.7) give the following knots for $\xi = 0(0.1)1$:

ξ	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
x	0	.28	.40	.49	.57	.63	.69	.75	.80	.85	1

Alternatively, assuming that the peak is at $x=0.5$ then the following knots are generated:

ξ	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
x	0	.2236	.3162	.3873	.4472	.5	.5250	.58	.68	.82	1

As a further illustration of this technique suppose that the initial condition of the partial differential equation has a peak at $x=\alpha$ and a trough at $x=\beta$. For such a condition, using functions of the type (5.4.4) and (5.4.7), (5.4.1) may be represented as

$$x = (\alpha\xi)^{\frac{1}{2}} \qquad x < \alpha \qquad\qquad (5.4.8)$$

$$x = \frac{2}{\beta-\alpha}(\xi-\alpha)^2 + \alpha \qquad \alpha < x < \frac{\alpha+\beta}{2} \qquad (5.4.9)$$

$$x = \left(\frac{\beta-\alpha}{2}\right)^{\frac{1}{2}}\left[\xi - \left(\frac{\alpha+\beta}{2}\right)\right]^{\frac{1}{2}} + \frac{\alpha+\beta}{2} \qquad \frac{\alpha+\beta}{2} < x < \beta \qquad (5.4.10)$$

$$x = \frac{1}{1-\beta}(\xi-\beta)^2 + \beta \qquad x > \beta \qquad\qquad (5.4.11)$$

with knots additionally positioned at both x=α and x=β.

However, suppose for example that the initial condition has the form

$$u(x,0) = \sin\pi x \qquad 0 \leqslant x \leqslant 1. \qquad\qquad (5.4.12)$$

Here one would expect the 'best' knots to be symmetrical about the peak x=0.5. The actual knots generated by the transformation (5.4.6) and (5.4.7) as given earlier, illustrate a drawback in this method. The major difficulty lies in generalising about the choice of the transformation function (5.4.1), while trying to take on board initial condition variations which cannot be explicitly bought into play.

Further discussion on the implementation of all three techniques described in this chapter is given in the following chapter on case studies.

CHAPTER 6

Case Studies 1

6.1   Case Study Philosophy

In this first chapter of case studies we assess the

effectiveness of the knot placement techniques derived

in the previous chapter. For various partial differential

equations, knot partitions are obtained from the methods

of sections 5.2 to 5.4; these are then employed to obtain

solutions using the schemes of chapter 4. The efficiency of

using non-uniform knot placings is assessed by making

comparisons with solutions produced for uniform knot partitions,

having a corresponding number of knots.

In obtaining results for the case studies of this chapter the

knots are chosen subject to the initial condition $g(x)$ and are

then fixed throughout time. This has the disadvantage that

if the solution to the partial differential equation changes

significantly in shape from that of the initial condition as time

progresses, the knots will no longer be in optimal positions.

6.2   Case Study 1.1

As an illustration of the application of spline techniques

in the numerical solution of hyperbolic partial differential

equations we first consider the simple wave equation (3.1.1)

with $a=1$, $b=c=0$

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} \qquad (0 \leqslant x \leqslant 1, \ t > 0) \qquad\qquad (6.2.1)$$

with the boundary conditions

$$u(0,t) = u(1,t) = 0 \qquad\qquad (6.2.2)$$

and the initial conditions

$$u(x,0) = \sin\pi x \qquad\qquad (6.2.3)$$

$$\frac{\partial u(x,0)}{\partial t} = 0 \ . \qquad\qquad (6.2.4)$$

To draw comparisons between the accuracy of the results produced using non-uniform knot partitions and constant knot spacings we require an equal number of knots in each case. For the constant knot spacing case we use h=0.1, which gives 9 internal knots in the range $\left[0,1\right]$.

Employing the initial condition (6.2.3) the recursive process (5.2.19) of the local method becomes

$$x_i = x_{i-1} + \left[\frac{384 \ \varepsilon}{\pi^4 \sin\pi x_{i-1}}\right]^{1/4} \qquad (i=1,2,\ldots,10) \qquad\qquad (6.2.5)$$

where ε is chosen to give 9 internal knots. An obvious problem in implementing (6.2.5) arises since the denominator is zero when x=0. This is easily overcome by fixing a knot at the peak x=0.5 and determining the knots from that point. Using the symmetry of (6.2.3) the internal knot positions produced are as shown in Table 1.

To determine suitable knots using the global method of section 5.3 the initial condition (6.2.3) is again employed, the integral expression (5.3.31) thus becoming

$$\pi \int_{x_i}^{x_{i+1}} (\sin\pi x)^{1/4} dx = \frac{\pi}{10} \int_0^1 (\sin\pi x)^{1/4} dx . \qquad (6.2.6)$$

$$(i=0,1,....,9)$$

The right hand side of (6.2.6) is initially evaluated using an IBM numerical integration routine employing the trapezoidal rule. The knots are then chosen so that the value of the integral between each pair of successive knots is arbitrarily close to one-tenth of the value of the integral between 0 and 1. This has been achieved using an interval halving technique which generates the knot positions which satisfy (6.2.6) to any desired accuracy, in this case taken to be 0.5×10^{-5}. The knots produced in this manner are again given in Table 1.

Further discussion on the application of both the local and global methods to this particular case study is given in Raggett and Wisher (1979a and 1979b).

The initial condition (6.2.3) obviously only has one peak in $x\epsilon[0,1]$, this being at x=0.5. The expressions (5.4.6) and (5.4.7) thus become, respectively

$$x_i = 2 (\xi_i - 0.5)^2 + 0.5 \qquad x > 0.5 \qquad (6.2.7)$$

and

$$x_i = (0.5\xi_i)^{1/2} \qquad\qquad x < 0.5 \qquad (6.2.8)$$

$$(i=0,1,....,10)$$

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The knot positions thus produced by the transformation method are also given in Table 1.

Equation (6.2.1) is now solved using the scheme (4.2.8) and the accuracy of the results produced using the three knot partitions shown in Table 1 are compared with results obtained using constant knot spacings. The accuracy is examined by evaluating the maximum absolute value of the error between the numerical solutions and the analytic solution, evaluated at each knot point, out to a chosen point in time. The analytic solution to the wave equation (6.2.1) with the prescribed boundary and initial conditions (6.2.2) and (6.2.3) is derived in Appendix 1 and is found to be

$$u(x,t) \quad = \quad \text{Sin}\pi x \, \cos\pi t. \hspace{3cm} (6.2.9)$$

Numerical solutions to (6.2.1) have been evaluated for a range of values of the parameter θ. Table 2(a) gives such results using a time step length of k=0.05, the errors being examined for 10 time steps out to t=0.5. Similarly, Table 3(a) shows maximum errors using k=0.01, in this case evaluated to t=0.1.

In certain more difficult problems the analytic solution may not be available and the accuracy of results obtained may be examined by evaluating the numerical value of the truncation error at each knot. This has been done for this particular

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case study and the maximum absolute values of the

trauncation error to fourth order derivative terms using k=0.05

are given for the various knot partitions in Table 4.

Results here are again for a range of θ values examined

for 10 time steps. As can be seen from Table 4 these results

suggest that the use of the local and global knot partitions

may prove advantageous to using constant knot spacing. The

truncation errors for the transformation knots are also

seen to be significantly larger than those of the other knot

partitions. This is because the order of truncation error

depends on k, h_i, h_{i+1} and from Table 1 it can be seen that

the distance between successive knots is relatively large

near x=0 and x=1. It should also be emphasised that due to the

changing nature of the derivative terms in the truncation

error this method of examining accuracy is unreliable and

is not employed in future case studies.

As suggested in section 3.1, the truncation error (4.2.15)

can be considerably simplified by choosing θ so that (3.1.20)

is satisfied. In this case, θ is thus chosen to be 1/12.

Extending this idea, it was earlier shown that for simple

problems involving only uniform knot partitions the parameter

θ can be chosen to eliminate the leading term of the truncation

error. This technique was examined in detail by Crandell (1955)

when using finite difference schemes for solving the heat

conduction equation. Further, Wisher (1977) suggested that

for schemes in which the knot partition is non-uniform, the

leading term of the truncation error can be eliminated

by suitably choosing θ at each knot point. When solving

the wave equation the truncation error (4.2.15) reduces to

$$k^2 \left[k^2 \left(\frac{1}{12} - \theta \right) + \frac{1}{12} \left(\frac{h_i^3 + h_{i+1}^3}{h_i + h_{i+1}} \right) \right] \frac{\partial^4 u}{\partial x^4} \quad + \ldots \qquad (6.2.10)$$

and thus to eliminate the fourth order term the parameter θ

should be chosen such that

$$\theta_i = \frac{1}{12} \left[1 + \frac{h_i^3 + h_{i+1}^3}{k^2 (h_i + h_{i+1})} \right] . \qquad (6.2.11)$$

Results using $\theta = 1/12$ and θ according to (6.2.11) are also

given in Tables 2(b) and 3(b).

In analysing the results given in Table 2(a) it is difficult

to draw any firm conclusions for this particular case study.

As can be seen, for $\theta \leqslant \frac{1}{3}$ the knot partitions produced using

both the local and global methods result in smaller errors than

when equally spaced knots are used. For $\theta > \frac{1}{3}$ the reverse

is true and the errors using constant knot spacings are smaller

than those for either the local or global methods. Considering

the results produced using the knots of the transformation

method, only when $\theta=1$ is any improvement seen, and this is

very marginal.

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The knots resulting from the transformation method also give numerical support to the stability condition (4.2.18). For example, when $\theta=0$, the scheme (4.2.8) is stable provided

$$k^2 \leq \frac{\min \{h_i h_{i+1}\}}{3} \quad . \qquad (6.2.12)$$

For the transformation knots given in Table 1, $\min\{h_i h_{i+1}\} = 0.001056$ and thus for stability we require

$$k^2 \leq 0.000352. \qquad (6.2.13)$$

Using k=0.05 this condition is violated and thus, as can be seen from Table 2(a), the results are unstable. If k=0.01, as in Table 3(a), then (6.2.13) is satisfied and stability is achieved.

As might be expected, the most accurate results for all choices of knots are produced when θ is chosen to remove the leading term of the truncation error. In fact, if θ is chosen subject to (6.2.11), the results produced using a uniform knot partition are superior to any of those using variable knot spacings. However, the results of Table 3(a), giving maximum errors only as far as t=0.1 using k=0.01, show that the local and global knot partitions give more accurate solutions than when using equally spaced knots. These results are consistent with the introductory remarks of this chapter.

6.3   Case Study 1.2

Here we again consider the simple one-dimensional wave

equation (6.2.1) with boundary conditions (6.2.2) but

choose the initial conditions to be

$$u(x,0) \;=\; x^4(1 - x) \tag{6.3.1}$$

and

$$\frac{\partial u}{\partial t}(x,0) = 0. \tag{6.3.2}$$

As shown in Figure 7, (6.3.1) is non-symmetrical in

$x\varepsilon\,[0,1]$ and is in fact a particular case of the Beta

probability distribution

$$f(x) = x^{\alpha-1}(1 - x^{\beta-1}) \qquad \alpha,\beta > 0 \;. \tag{6.3.3}$$

The initial condition (6.3.1) is again employed to determine

non-uniform knot partitions using both the local and global

techniques of chapter 5. The recursive relationship (5.2.19)

of the local method and the integral expression (5.3.31)

from the global method respectively become

$$x_i = x_{i-1} + \left[\frac{384\varepsilon}{\big|24 - 120x_{i-1}\big|}\right]^{1/4} \qquad (i=1,2,\ldots,10) \tag{6.3.4}$$

and

$$\int_{x_i}^{x_{i+1}} \big|24 - 120x\big|^{1/4}\, dx = \frac{1}{10}\int_{0}^{1} \big|24 - 120x\big|^{1/4}\, dx \;. \tag{6.3.5}$$
$$(i=0,1,\ldots,9)$$

The knots produced by evaluating each of the expressions
(6.3.4) and (6.3.5) are given in Table 5. These knot
partitions and uniformly spaced knots with h=0.1 are now
used in (4.2.8) producing solutions for this case study.
Comparisons in accuracy are again made by evaluating the
maximum absolute value of the error between the numerical
solutions and the following Fourier series analytic solution
(derived in Appendix 2)

$$u(x,t) = \sum_{n=1}^{\infty} 2\left[\frac{24}{(n\pi)^5} - \left(\frac{-8}{(n\pi)^3} + \frac{96}{(n\pi)^5}\right) \cos n\pi\right] \text{Sin} n\pi x \cos n\pi t.$$

(6.3.6)

Results given in Table 6(a) show these maximum errors for
k=0.05 using a range of θ values. The errors have again been
examined for 10 time steps out to t=0.5. The results show
that when θ=0 and θ=1/4 the errors produced using the local
and global knots are smaller than those using equally spaced
knots, the results of the global method being superior. However,
for the remaining θ values used constant knot spacing proves
more accurate. The results of Table 6(a) are therefore again
inconclusive. Overall, as can be seen in Table 6(b), the errors
of smallest magnitude occur when θ is chosen to remove the
leading term of the truncation error when the knots of the
local method are used.

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These rather inconclusive results can best be explained by

graphing the analytic solution (6.3.6) for various time

levels. As can be seen in Figure 7 the peak of the solution

moves in the x direction as time progresses and by t=0.5

the shape of the wave is completely different from its original

initial condition (6.3.1). The local and global knot partitions

are thus no longer optimally placed. We would, however,

expect the local and global knots to give improved accuracy

close to the initial line t=0 since for small t the shape

of the solution is very close to that of the initial condition.

As can be seen in Table 7 this is in fact found to be the case.

Further numerical evidence of this is given in Table 8 where

the maximum errors are listed using k=0.01 for 10 time steps.

These results show that for all the θ values used the solutions

produced using the local and global knot partitions always

have smaller errors than when uniformly spaced knots are

employed. However, the above reasoning is contradicted by

the results shown in Table 9 where maximum errors are again

given using k=0.01. In this case the errors are examined for

50 time steps out to t=0.5 and as can be seen, the local and

global knots still prove more accurate. While this result

is somewhat surprising, it is also gratifying that the

proposed new methods seem to be an improvement on constant

knot spacing when the time steps are chosen relatively small.

6.4   <u>Case Study 1.3</u>

As a final illustration of the use of spline techniques

for solving hyperbolic partial differential equations we

assume that the coefficients a and b in (3.1.1) have the

values unity and zero respectively, and thus the equation

under consideration is

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} + cu \quad . \quad (0 \leq x \leq 1, \ t > 0) \tag{6.4.1}$$

Equation (6.4.1) is assumed to be subject to the boundary

conditions (6.2.2) and the initial conditions (6.2.3) and (6.2.4).

The analytic solution to (6.4.1) is as derived in Appendix 3

and is given by

$$u(x,t) = \text{Sin}\pi x \cos(\pi^2 - c)^{1/2} t. \tag{6.4.2}$$

To examine the effect of the lower order term cu, various values

of the coefficient c are used, although in each case c is

chosen to be negative to avoid any occurrence of negative

square roots in (6.4.2).

As in previous case studies, numerical solutions are obtained

using constant knot spacing with h=0.1 and also using the

knot partitions resulting from the local and global methods

of chapter 5. Since the initial condition used here is the same as that employed in case study 1.1, the knots resulting from the local and global methods are again as given in Table 1. As previously, accuracy is examined by evaluating the maximum absolute error between the numerical solutions and the analytic solution (6.4.2) at the knots out to a certain point in time. Results given in Tables 10 and 11 show maximum errors for a range of values of c using k=0.05 and k=0.01 respectively. In each case results are examined out to t=0.5 and the parameter θ is chosen as $\frac{1}{3}$. The errors given in Table 10 show that only when c=-1 do the variable knot spacings prove superior to constant knot spacing. In Table 11, increased accuracy is observed when the local and global knot partitions are used for both c=-1 and c=-10.

As can be seen in both Tables 10 and 11, for large negative values of c, the errors resulting from the use of all knot partitions are large in magnitude and no improvement is gained by employing non-uniform knot spacings. It should however be noted that since the coefficient c in (6.4.1) is effectively multiplied by k^2 then, particularly for large negative values of c, as k is decreased in size the accuracy of the results obtained increases.

The equation (6.4.1) is also useful for assessing the effect of lower order terms on the stability of the scheme (4.2.8). Various authors (see for example Fox (1962), Richtmyer and Morton (1967) and Griffiths (1982)) have suggested that it is reasonable to assume that the presence of the lower order terms, $b\frac{\partial u}{\partial x}$ and cu, have no great effect on the stability condition of a particular finite difference scheme. In section 4.2 it is shown that the stability of the scheme (4.2.8) is unaffected by the presence of a cu term in (3.1.1) and that the scheme (4.2.8) is unconditionally stable when $\theta \geqslant \frac{1}{4}$. This is confirmed by the results of Tables 10 and 11. Further, when $\theta < \frac{1}{4}$, the scheme (4.2.8) is stable provided that the condition (4.2.18) is satisfied. For this case study, when equally spaced knots are employed for example, the condition (4.2.18) reduces to $\theta \geqslant -\frac{1}{12}$ when k=0.05. The results shown in Table 12 are produced when the parameter θ is chosen to be zero and, as can be seen, stability is still achieved.

6.5   Case Study 1.4

In this case study we illustrate the application of the spline scheme derived in section 4.3 for obtaining numerical solutions to parabolic partial differential equations. We consider the simple one-dimensional heat conduction equation ((3.3.1) with a=1, b=c=0)

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \qquad (0 \leq x \leq 1, \ t > 0) \qquad (6.5.1)$$

together with the initial condition

$$u(x,0) = \sin\pi x \qquad (6.5.2)$$

and the boundary conditions

$$u(0,t) = u(1,t) = 0 \ . \qquad (6.5.3)$$

As in previous case studies, solutions are obtained using
9 internal knots and thus in the equally spaced knot case,
h=0.1 is used. Since the initial conditions (6.5.2) and
(6.2.3) are the same, the knots of the local and global
methods are again given by (6.2.5) and (6.2.6) respectively.
These knot positions are given in Table 1. Numerical solutions
to (6.5.1) subject to (6.5.2) and (6.5.3) have been obtained
employing the knots of Table 1, solutions being derived using
the spline scheme (4.3.1). As shown in Appendix 4, the
analytic solution for this case study is given by

$$u(x,t) = e^{-\pi^2 t} \sin\pi x \ . \qquad (6.5.4)$$

The results given in Table 13(a) are the maximum absolute
values of the errors between the numerical solutions and the
analytic solution (6.5.4) using a time step length of k=0.05,
results being examined for 10 time steps. As can be seen the
errors produced using all three knot partitions are very
similar in magnitude. The only case when the use of variable

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knot spacings gives improved accuracy over constantly

spaced knots is when the parameter θ is chosen to be 1/2.

It should be noted, however, that this value of θ is the

most suitable choice when no additional information is

available since it gives equal weighting to both time

levels. The results of Table 14(a), where maximum errors

for 50 time steps (using k=0.01) are given, confirm this.

Results produced using θ=1/4 are included to provide

numerical evidence to the stability condition (4.3.4). For

example, using the local knots (4.3.4) is satisfied provided

$\theta \geqslant 0.486$ when k=0.05 is used and provided $\theta \geqslant 0.430$ in the

case of k=0.01.

As suggested in section 6.2, in certain instances the leading

term of the truncation error may be eliminated by suitable

choice of the parameter θ. For this particular case study

the truncation error is given by (4.3.3) and thus by choosing

θ such that

$$\theta_i = \frac{1}{2} + \frac{1}{12k} \left(\frac{h_i^3 + h_{i+1}^3}{h_i + h_{i+1}} \right) \tag{6.5.5}$$

the fourth order derivative term is reduced to zero. Results

obtained using (6.5.5) are given in Tables 13(b) and 14(b).

In both cases the errors resulting from the use of the local

and global knot partitions are smaller than those when
equally spaced knots are employed. In addition, as might
be expected, choosing θ from (6.5.5) results in the most
accurate solutions obtained.

6.6   Case Study 1.5

As a final illustration of the suitability of the local and
global methods we again consider the heat conduction equation
(6.5.1). In this case study we assume (6.5.1) has the initial
condition

$$u(x,0) \;=\; e^{-ax} \tag{6.6.1}$$

and the boundary conditions

$$u(0,t) = 1 \tag{6.6.2}$$

and $u(1,t) = e^{-a} \tag{6.6.3}$

where a is a constant > 0. Since we again choose to have 9
internal knot points in $x \in [0,1]$ the knots of the local method
are given by the recursive process

$$x_i \;=\; x_{i-1} \;+\; \left[\frac{384\varepsilon}{a^4 e^{-ax_i}} \right]^{1/4} \quad (i=1,2,\ldots,10) \tag{6.6.4}$$

Similarly, applying the global method of section 5.3 the knot
partition results from the following expression

$$\int_{x_i}^{x_{i+1}} \left(a^4 e^{-ax}\right)^{1/4} dx = \frac{1}{10} \int_o^1 \left(a^4 e^{-ax}\right)^{1/4} dx. \qquad (6.6.5)$$

$$(i=0,1,\ldots,9)$$

In carrying out numerical computations we have chosen the constant a to take the values 1 and 10. The shapes of the initial condition (6.6.1) using these values of a are shown in Figure 8. The knot partitions resulting from the expressions (6.6.4) and (6.6.5) using a=1 and a=10 are given in Tables 15 and 16 respectively.

As in the previous case studies we assess the usefulness of the local and global methods by comparing the results produced using these knots with results obtained using equally spaced knots. For this particular case study the analytic solution, which is derived in Appendix 5, is given by

$$u(x,t) = \left[1 + (e^{-a} -1)x\right]$$

$$+ \sum_{n=o}^{\infty} \frac{2}{n\pi} (e^{-a}\cos n\pi - 1)\left(\frac{a^2}{(n\pi)^2 + a^2}\right)\operatorname{Sin}n\pi x e^{-n^2\pi^2 t}$$

$$(6.6.6)$$

This analytic solution is evaluated at each knot point and the accuracy is again examined by calculating the maximum absolute error between the numerical solution and the analytic solution (6.6.6) for a chosen number of time levels.

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For the case when the constant a is chosen to be unity

Tables 17(a) and 18(a) show the maximum errors using k=0.05
and k=0.01 respectively. Similarly, when a=10 the maximum
errors obtained are given in Tables 19(a) (for k=0.05) and
20(a) (for k=0.01). In all computations the errors have been
examined out to t=0.5.

Analysing the results for a=1 first, we see that, as in
the previous case study, only when $\theta = \frac{1}{2}$ do the non-uniform
knot partitions result in smaller errors than when uniformly
spaced knots are used. This is the case for both k=0.05 and
k=0.01. Again the choice of $\theta = \frac{1}{2}$, which gives equal weighting
to each of the time levels, is a logical choice without
prior knowledge which may result in increased accuracy.
It should however be noted that the errors resulting from
each of the knot partitions are very similar in magnitude
for individual θ values.

As in case study 1.4, θ may be chosen to remove the leading
term of the truncation error (4.3.3). Again this is done by
choosing the parameter θ from the relationship (6.5.5). As
is shown in Tables 17(b) and 18(b), this choice of θ results
in the most accurate solutions obtained for each of the knot

partitions for both k=0.05 and k=0.01. However, using

this value of θ the local and global knots only result

in smaller maximum errors when the time step length

k=0.05. When k=0.01 constant knot spacing is more accurate.

Considering now the case when a=10, the maximum errors

resulting from uniformly spaced knots are always smaller in

magnitude than those when variable knot spacings are employed

if k=0.01. When a time step length of k=0.05 is used,

$\theta = \frac{1}{2}$ is again the only case where the local and global

methods give any improvement. This includes choosing the

parameter θ such that the leading term of the truncation

error is removed.

It is worthwhile to here consider in more detail the results

obtained when the constant a in (6.6.1) is equal to ten.

For this value of a the analytic solution (6.6.6) has the

form shown in Figure 9 for various time levels. As can be

seen, the shape of the analytic solution becomes less 'severe'

as time progresses and by t=0.5 the solution is approximately

linear. The knots produced using the local and global methods

will therefore not be optimally placed for large t. As in

case study 1.2, it might be expected that the local and global

knot partitions give improved accuracy close to the initial

line t=0. We have however found that close to t=0 the numerical

solutions oscillate either side of the analytic solution

for successive time lines and that the maximum errors

quoted in Tables 19 and 20 always occur on the second

time line; improvement is therefore not observed in this

case.

CHAPTER 7

Varying the Knots on Each Time Line

7.1   Preamble

In the case studies of Chapter 6 numerical solutions

are obtained using knot partitions which are derived subject

to the initial condition g(x) of the partial differential

equation. These knots are then fixed throughout time. As

was seen in case studies 1.2 and 1.5, when the shape of

the solution to the partial differential equation changes

significantly as time progresses then the knots will no

longer be optimally placed. It would therefore be desirable

to have an algorithm in which optimal knot partitions are

derived on each time line. Obviously, if the position of

the mesh points in any finite difference scheme change on

each time line, then that scheme becomes much more complex

(see for example, Murray and Landis (1959), where such a

scheme was used in the solution of moving boundary problems

in heat flow). Fortunately, in using spline functions, an

interpolating polynomial is available which can be used to

obtain solutions at points intermediate to the existing

knot points.

The technique used in the following section to determine

a new partition of optimal knots on each new time line,

is based on the previously described global method and is

an extension of the work of Dobson (1972) who used spline

techniques in approximation problems. As was shown in

section 5.3, the optimal knot partition of the global

method results from the integral expression (5.3.30). This

expression requires knowledge of the fourth derivative

of the function $f(x)$ with respect to x. In the case studies of

Chapter 6, $f(x)$ was taken to be the given initial condition.

If the global method is used as a basis for generating new

knots on each new time line then $f(x)$ will be unknown as

time progresses. This problem can be overcome by making

use of the spline function $S(x)$ as given by (4.2.1). It

would therefore seem reasonable to approximate $f^{iv}(x)$ in

(5.3.30) by $S^{iv}(x)$. However, since in this work we use

cubic splines, then only the first and second derivatives

are continuous and $S^{iv}(x) = 0$ in each knot interval. This

problem is overcome using the following algorithm.

7.2   Procedure for Determining Optimal Knot Partition

Assume that a partition of knots π_j (as defined in (3.1.4))

and the corresponding numerical solutions $u_{i,j}$ at these

knots are known on the jth time line. On the initial line,

the knots π_o can either be taken as equally spaced or

obtained using one of the methods of Chapter 5.

(i)　　Determine the mid-points of the knots of π_j,

$$x_{i-\frac{1}{2}} = \frac{x_{i-1} + x_i}{2} \qquad (i=1,2,\ldots,N) \qquad (7.2.1)$$

(ii)　　Evaluate the third derivative of the spline function at the mid-points from the relationship

$$S_j'''(x_{i-\frac{1}{2}}) = \frac{1}{h_i}(M_{i,j} - M_{i-1,j}) \qquad (7.2.2)$$

$$(i=1,2,\ldots,N)$$

the $M_{i,j}(i=0,1,\ldots,N)$ first being determined

from (4.2.2) with $M_{0,j} = M_{N,j} = 0$.

(iii) Obtain an approximation to $S_j^{iv}(x)$ at the knots x_i,

$$S_j^{iv}(x_i) = \frac{S_j'''(x_{i+\frac{1}{2}}) - S_j'''(x_{i-\frac{1}{2}})}{x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}} \qquad (i=1,2,\ldots,(N-1))$$

$$(7.2.3)$$

where the $S_j^{iv}(x_i)$ will be piecewise constants with

discontinuities at the mid-points $x_{i-\frac{1}{2}}$.

While we realise that this is a crude approximation

$(S_j^{iv}(x)$ is not well-defined at the knots), this procedure

has been used with success by Dobson (1972) and

de Boor (1978).

(iv) Compute the values of

$$\left| S_j^{iv}(x_i) \right|^{1/4} \qquad (i=1,2,\ldots,(N-1)). \qquad (7.2.4)$$

These will have the form illustrated in Figure 10, the functions $\left| S_j^{iv}(x_1) \right|^{1/4}$ and $\left| S_j^{iv}(x_{N-1}) \right|^{1/4}$ being extended to include all the range $[0,1]$.

(v) Using the expression (5.3.30) the new knots $x_i'(i=0,1,\ldots,N)$ on the jth time line should thus be chosen such that

$$\int_{x_i'}^{x_{i+1}'} \left| S_j^{iv}(x) \right|^{1/4} dx = \frac{1}{N} \int_0^1 \left| S_j^{iv}(x) \right|^{1/4} dx. \quad (7.2.5)$$

$$(i=0,1,\ldots,(N-1))$$

The right-hand-side of the integral expression (7.2.5) is evaluated by summing the areas of the rectangles shown in Figure 10.

The relationship (7.2.5) thus becomes

$$\int_{x_i'}^{x_{i+1}'} \left| S_j^{iv}(x) \right|^{1/4} dx = A_S \qquad (7.2.6)$$

where the constant A_S is given by

$$A_S = \frac{1}{N} \left\{ \left| S_j^{iv}(x_1) \right|^{1/4} \cdot x_{\frac{1}{2}} + \sum_{i=1}^{N-1} \left| S_j^{iv}(x_i) \right|^{1/4} (x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}) \right.$$

$$\left. + \left| S_j^{iv}(x_{N-1}) \right|^{1/4} (1 - x_{N-\frac{1}{2}}) \right\} .$$

$$(7.2.7)$$

The knots are thus determined using the following

procedure. Assume that a knot x_i' has been determined, as

illustrated in Figure 11. The knot x_{i+1}' is found as

follows:

(a) Evaluate

$$A_n = \left| S_j^{iv}(x_M) \right|^{1/4} (x_{M+\frac{1}{2}} - x_i')$$

and let $A_L = 0$.

(b) If $A_n > A_S$, then

$$x_{i+1}' = x_i' + \frac{A_S - A_L}{\left| S_j^{iv}(x_M) \right|^{1/4}}$$

(c) If $A_n = A_S$, then

$$x_{i+1}' = x_{M+\frac{1}{2}}.$$

(d) If $A_n < A_S$, then let

$$x_i' = x_{M+\frac{1}{2}},$$

$$A_L = A_n$$

and $M = M+1$.

Evaluate

$$A_n = A_n + \left| S_j^{iv}(x_M) \right|^{1/4} (x_{M+\frac{1}{2}} - x_{M-\frac{1}{2}})$$

and return to (b).

As previously mentioned, this technique has been used

by Dobson (1972), in approximating a function f by

splines of various order. In that work, the author

performed several iterations of the algorithm and

examined the errors produced using the knots of each

iteration. It was found that only one or two iterations

were usually required, after which no improvement in

accuracy was gained. As shown in the following section,

we here perform only one iteration of the knot placement

algorithm per time line, since with several iterations

the process becomes computationally expensive. However,

in the following chapter on case studies, it is noticed

that certain conditions on the size of the time step length,

and hence on the relative position of the knot partitions,

should be observed.

7.3   Implementation of the Splines Schemes

With knots varying on each time line, numerical solutions

to a given partial differential equation are again to be

derived using the splines schemes (4.2.8) for hyperbolic

equations and (4.3.1) for parabolic equations. In the

case of hyperbolic partial differential equations the

implementation of (4.2.8) is accomplished as follows:

Assume that the scheme is fully developed in that

solutions $u_{i,j}$ ($j\geqslant1$) are known on the time lines

t=o to t=jk. Using the algorithm described in section

7.2, a new partition of knots π_j is obtained. Solutions

$u_{i,j-1}$ and $u_{i,j-2}$ at these spatial knots are found

using the spline function (4.2.1), these being used

in (4.2.8) to determine new solutions $u_{i,j}$. The scheme

(4.2.8) is employed again to find solutions $u_{i,j+1}$,

the process then being repeated. As previously stated,

on the initial line the knots π_o are chosen to be equally

spaced or derived using one of the methods of Chapter 5.

Employing the derivative initial condition of (3.1.3),

solutions $u_{i,1}$ are found from (4.2.8). A new partition

of knots π_1 is then obtained from the algorithm of

section 7.2. Solutions $u_{i,o}$ at these knots are found from

the initial condition (3.1.3), these being used in (4.2.8)

to determine new solutions $u_{i,1}$. The scheme (4.2.8) is

employed again to determine $u_{i,2}$, the process then being

fully developed.

In the case of parabolic partial differential equations

the procedure is as above but is simplified since the

scheme (4.3.1) is only two time level. Having found a

new partition of knots π_j, the spline function (4.2.1)

is required only once, this being to obtain solutions

$u_{i,j-1}$ at these knots on the previous time line.

CHAPTER 8

Case Studies 2

8.1   Case Study Philosophy

Here we again consider each of the case studies of

Chapter 6 and derive solutions by choosing optimal knot

partitions on each time line using the technique described

in the previous chapter. The application of the technique

to both hyperbolic and parabolic partial differential

equations is therefore considered. Results obtained by

varying the knots on each time line are compared with

both those resulting from constantly spaced knots and the

knots of the local and global methods. In the tables referred

to in the following case studies, the results obtained in

Chapter 6 are therefore listed again to enable comparisons

to be made.

It should be noted that in sections 6.3 and 6.6 it was

suggested that, due to the changing nature of the solution

of the respective partial differential equations', improvement

might be expected from a scheme in which optimal knots are

chosen on each new time line.

8.2   Case Study 2.1

The simple one-dimensional wave equation (6.2.1) subject

to (6.2.2), (6.2.3) and (6.2.4) is reconsidered here.

Using the algorithm described in section 7.2, optimal

knot partitions are derived on each time line and solutions

obtained employing the procedure of section 7.3. To enable

comparisons to be made with the results of case study 1.1,

9 internal knots are chosen on each time line and solutions

are obtained for a range of values of the parameter θ.

Accuracy is again examined by evaluating the maximum absolute

difference between the numerical solutions and the analytic

solution (6.2.9) at the knots, out to a chosen point in time.

The errors given in Table 21 are those obtained using a

time step length of k=0.05, results being examined out to

t=0.5. As can be seen, for $\theta \leq \frac{1}{3}$ results produced by varying

the knots on each time line are an improvement on results

obtained using equally spaced knots. However, the errors of

smallest magnitude are observed when the knots of the earlier

described global method are employed. When $\theta > \frac{1}{3}$, using

equally spaced knots gives greatest accuracy.

The results of Table 21 suggest that for this particular case study no improvement in accuracy is to be gained by varying the knots on each time line. This might be expected since, as can be seen from (6.2.9), the solution has the form of a symmetrical wave. Figure 12 shows the partitions of knots derived using the algorithm of section 7.2 for certain time lines when the parameter θ is chosen to be $\frac{1}{3}$. As can be seen, little variation in the knot partitions is observed as time progresses and thus, due to the additional computation required, no increase in accuracy is obtained by varying the knots on each time line.

8.3   Case Study 2.2

Here we again consider case study 1.2 and derive solutions to the hyperbolic partial differential equation (6.2.1) with boundary conditions (6.2.2) and initial conditions (6.3.1) and (6.3.2).

Using the technique described in Chapter 7 solutions are obtained, the algorithm being employed to produce 9 internal knots on each time line. The results given in Table 22 are the maximum absolute errors between the numerical solutions and the analytic solution (6.3.6), where results were examined out to t=0.5 using a time step length of k=0.05.

As mentioned earlier, and illustrated in Figure 7, the analytic solution (6.3.6) is such that the peak of the wave moves in the x direction as time progresses. We would therefore hope that by varying the knots on each time line some improvement in accuracy would be observed. The results given in Table 22 show that this is not the case for this particular choice of k. As can be seen, for all choices of the parameter θ the errors produced by varying the knots on each time line are always larger in magnitude than those resulting from either uniformly spaced knots or from the variable knot spacings of the local and global methods.

To further test the algorithm, solutions were derived using a time step length of k=0.01; again 9 internal knot points were used. The results shown in Table 23 are the maximum absolute errors between the numerical solutions and the analytic solution (6.3.6) using k=0.01 in which errors were examined at the knot points for 50 time steps out to t=0.5. In this case the errors produced by varying the knots on each time line are considerably smaller than those obtained earlier in case study 1.2. For all choices of the parameter θ shown, the results obtained by varying the knots on each

time line are always more accurate than those produced

by using either constant knot spacing or the knots of

the local and global methods. By using a small time step

length we thus see that significant improvement is gained

by choosing different knot partitions on each time line.

Some explanation of the above can be obtained by examining

the positions of the knots resulting from the application

of the knot placement algorithm for each choice of step

length k. Figures 13 and 14 show the partitions of knots

produced by the algorithm on certain time lines when

k=0.05 and k=0.01, respectively. Comparing these partitions

with the shape of the analytic solution shown in Figure 7,

we see that when k=0.01 the knots marginally better match

the changing nature of the analytic solution than those

derived when k=0.05, particularly on the early time lines.

The situation is further clarified when more than 9 internal

knot points are produced on each time line. Figures 15 and

16 show the partitions of knots produced when 19 internal

knots are allowed and the time step length is chosen to be

k=0.05 and k=0.01, respectively. As can be seen, considerable

improvement in the positioning of the knots is obtained when

the smaller step length k=0.01 is used. When k=0.05, the

knots resulting from the application of the knot placement

algorithm given in section 7.2 remain 'bunched' close to

x=1 and do not match the analytic solution (6.3.6).

Additionally, Figure 17 shows the knots produced by the

algorithm on t=0.5 when the analytic solution (6.3.6) is

used instead of the numerical solutions. This has been

done for comparison purposes and it is interesting to note

that the knots produced in this way are very similar to

those in Figure 16 when k=0.01 was used.

We thus here conclude that improvement in accuracy is to be

gained by varying the knots on each time line if a small time

step length is employed.

8.4   Case Study 2.3

In this section we reconsider case study 1.3 and derive

solutions to equation (6.4.1) by producing different knot

partitions on each time line. To enable comparisons to be

made with earlier obtained results we again choose 9 internal

knots on each time line and obtain solutions for various

negative values of the coefficient c.

The results given in Tables 24 and 25 are the maximum absolute

errors between the numerical solutions and the analytic

solution (6.2.4) out to t=0.5 using time step lengths

of k=0.05 and k=0.01, respectively. All results shown

have again been obtained when the parameter θ is taken to

be $\frac{1}{3}$. Examining the errors given we see that for both

choices of k, no improvement in accuracy is observed by

using different knot partitions on each time line. In

certain instances (namely, c=-1 when k=0.05 and c=-1,

c=-10 when k=0.01) the errors produced by varying the knots

on each time line are smaller than those resulting from

equally spaced knots. However, in each of these cases, the

results derived using either the local or global knot

partitions are a further improvement. If the coefficient

c is chosen to be -100 or -200, the errors for k=0.05

are almost identical for each of the methods presented.

When the time step length k is taken to be 0.01, Table 25

shows that, for these large values of c, constant knot

spacing gives greatest accuracy.

When considering the results obtained by choosing different

knot partitions on each time line it should be noted that

the analytic solution (6.4.2) is symmetrical in [0,1] for

all values of the coefficient c. As was seen in case study

2.1, little benefit is therefore gained by varying the knots

at each stage in time.

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8.5   <u>Case Study 2.4</u>

In this case study we now apply the technique described

in Chapter 7 to parabolic partial differential equations.

We again consider the one-dimensional heat conduction

equation (6.5.1) subject to the initial condition (6.5.2)

and the boundary conditions (6.5.3). The algorithm given

in section 7.2 is again used to produce 9 internal knot

points on each time line and these are employed in the

scheme (4.3.1) using the technique described in section 7.3.

Figure 18 shows the partitions of knots produced by the

algorithm on certain time lines when the parameter θ is

chosen to be $\frac{1}{2}$ and when a time step length of k=0.05 is

used.

The results shown in Tables 26 and 27 are the maximum errors

between the numerical solutions and the analytic solution

(6.5.4) using k=0.05 and k=0.01, respectively. Results

have been examined at the knot points, out to t=0.5 in each

case. As can be seen, for both choices of k, the errors

obtained by varying the knots on each time line are smaller

than those resulting from both uniformly spaced knots and

the knots of the local method when $\theta = \frac{1}{2}$. However, in

each case further improvement is obtained by using the knots

of the global method. For $\theta > \frac{1}{2}$, using a constant knot spacing

of h=0.1 proves most accurate for both k=0.05 and k=0.01.

For this particular parabolic partial differential equation the analytic solution (6.5.4) has a symmetrical form for all time with the solution dying out as time progresses. As shown in Figure 18 the knot partitions produced in this case study are very similar on each time line and are approximately constantly spaced. Little is therefore to be gained by varying the knots on each time line.

8.6   ## Case Study 2.5

Here we reconsider the parabolic partial differential equation (6.5.1) together with the initial condition (6.6.1) and the boundary conditions (6.6.2) and (6.6.3). To enable comparisons to be made with the results obtained in case study 1.5 we again let the constant a in (6.6.1) take the values 1 and 10. In each case, solutions have been derived by using the algorithm in section 7.2 to produce new knot partitions on each time line. The accuracy of the solutions obtained is examined by comparing them with the known analytic solution (6.6.6) at each knot point. The results given in Tables 28 and 29 are the maximum absolute errors between the numerical solutions and the analytic solution when the constant a is equal to 1 and time step lengths of k=0.05 and k=0.01, respectively, are used.

Similarly, the results shown in Tables 30 and 31 are the maximum errors produced using k=0.05 and k=0.01, respectively, when a is chosen to be 10. Errors in all tables have been examined out to t=0.5. In addition, Figures 19 to 22 show the partitions of knots generated by the knot placement algorithm for both a=1 and a=10 using time step lengths of k=0.05 and k=0.01. In each case, 9 internal knots are chosen on each time line and the partitions produced are those when the parameter θ is taken to be $\frac{1}{2}$.

Examining the results for a=1 first, we see from Table 28 that when $\theta = \frac{1}{2}$ and $\theta = \frac{3}{4}$ the results obtained by varying the knots on each time line are an improvement over those produced using either equally spaced knots or the knots of the local and global methods. In the case when θ is chosen to be unity, constant knot spacings prove most accurate. When k=0.01, Table 29 shows that for $\theta = \frac{1}{2}$ the errors resulting from varying the knots on each time line are smaller than those for each of the other knot partitions used. When $\theta = \frac{3}{4}$ and $\theta = 1$, using equally spaced knots again results in the smallest errors. The results of Tables 28 and 29 are encouraging since the choice of $\theta = \frac{1}{2}$ is the most suitable in that it gives equal weighting to each of the time lines in the scheme (4.3.1).

We now turn our attention to the results produced

when the constant a in (6.6.1) is equal to 10. As can

be seen from Table 30, when the time step length k=0.05

is employed smaller errors result by choosing different

knot partitions on each time line than by using either

equally spaced knots or the knots of the local and global

methods when θ is set to $\frac{1}{2}$. The results for $\theta = \frac{3}{4}$ and

$\theta = 1$ again show that constantly spaced knots are most

accurate. In the case when k=0.01, the results of Table 31

show that the smallest errors for all choices of the

parameter θ are produced by choosing the knots to be

equally spaced.

The results for a=10 are surprising if one considers the

distributions of knots produced by the knot placement algorithm

for both k=0.05 and k=0.01. Figures 21 and 22 indicate that

more reasonable paritions of knots are produced when the

smaller time step k=0.01 is employed (see figure 9 for

analytic solution) since the knots for k=0.05 remain 'bunched'

close to x=o for all time. These partitions of knots are

consistent with those produced in case study 2.2 where a

small time step length again gave better partitions.

However, the results of Table 31 show that no

improvement in accuracy is gained by varying the knots on

each time line when k=0.01 is used. The reason for this,

as indicated in case study 1.5, is because close to t=o

the numerical solutions oscillate either side of the analytic

solution and the maximum error always occurs on the second

time line for any choice of knots used. The benefit from

the more reaslistic knot partitions is therefore not

realised.

CHAPTER 9

Conclusions and Extensions

9.1   Conclusions

Before drawing general conclusions about the proposed

methods we here first briefly review the results obtained

in the earlier case studies. This may repeat some of the

comments made in chapters 6 and 8 but will enable easier

comparisons.

In case studies 1.1 and 2.1 we considered the one-dimensional

wave equation having a symmetric initial condition. The

results obtained showed that for the smaller values of the

parameter θ used, the knots of the global method gave

greatest accuracy. For larger θ values, using equally spaced

knots resulted in the relatively smaller errors. In certain

cases, varying the knots on each time line produced greater

accuracy than equally spaced knots, although in these cases

the errors were still larger than those resulting from the

knots of the global method. For this case study, without

any additional information, the value $\theta = 1/3$, is the most

logical a priori choice since it gives equal weighting to each

of the time lines in the scheme (4.2.8) used. For this

particular θ value the global knot partition results in

greatest accuracy. Employing the knots of the global

method is therefore advantageous in this case. As mentioned

earlier, due to the symmetrical initial condition, no overall

improvement in accuracy is gained here by varying the knots

on each of the time lines.

The one-dimensional wave equation was again considered in

case studies 1.2 and 2.2. In this case the initial condition

was chosen to be non-symmetrical and resulted in a wave form

in which the peak of the wave moves in the x direction as

time progresses. From the results obtained it was found that

the knots of the local and global methods gave increased

accuracy in certain cases, particularly for small time step

lengths k. Since the wave form moves as time progresses it

was noted that the local and global knot partitions, being

based on the initial condition, would no longer be optimally

placed away from the initial line. The results obtained by

choosing different optimal knot partitions on each time line

showed that, for a larger time step length of k=0.05, no

improvement in accuracy over the use of local or global knots

was observed; moreover in only one instance were the errors

smaller than those of constant knot spacing. However, when

a smaller time step length of k=0.01 was employed, the

technique of varying the knots on each time line produced

a significant increase in accuracy. For all θ values used,

the errors resulting from these knot partitions were always

considerably smaller in magnitude than those of either

equally spaced knots or the knots of the local and global

methods.

A final example on the application of the techniques to

hyperbolic partial differential equations was discussed in

case studies 1.3 and 2.3. Here the constants a and b in

(3.1.1) were chosen to be unity and zero respectively,

whilst the coefficient c was allowed to take various negative

values. The results obtained indicate that for smaller

negative values of c, some improvement in accuracy over

equally spaced knots is to be gained by using either the

local or global knot partitions. In some instances, the

errors produced by varying the knots on each time line are

also smaller in magnitude than constant knot spacing, although

a further reduction in the magnitude of the errors is always

produced by employing the local or global knots. This is to

be expected since the initial condition used in this case

study is again symmetrical. For larger values of the

coefficient c, the magnitude of the errors increases with

little to choose between the results of the various knot

partitions.

In case studies 1.4 and 2.4 we considered the one-dimensional heat conduction equation, again choosing the initial condition to be symmetrical in shape. The results derived showed that when the parameter $\theta = 1/2$, the errors produced by varying the knots on each time line are smaller in magnitude than the errors resulting from uniformly spaced knots. However, as previously, the results of either the local or global knot partitions give a further improvement in accuracy. For the remaining θ values used, constantly spaced knots proves most accurate. It should however be noted that the choice of $\theta=1/2$ gives the natural 'Crank-Nicolson like' equal weighting to each of the time lines in the scheme (4.3.1) and for this value of θ the global knots result in the most accurate solutions. Due to the symmetrical shape of the solutions little is again gained by choosing different knots on each of the time lines.

The final partial differential equation considered was that of case studies 1.5 and 2.5, in which the heat conduction equation was assumed to have an exponential initial condition with the parameter being chosen to be a=1 and a=10. For a=1, the results produced by varying the knots on each time line

are superior to those found using equally spaced knots,
or the knots of the local or global methods when θ is
chosen to give equal weighting to each of the time lines.
A similar improvement is gained by using $\theta=3/4$ when the
time step length is k=0.05, although for the remaining
values of θ and k equally spaced knots results in the errors
of smallest magnitude. These encouraging results are not
observed when the parameter a equals 10. In this case, only
when $\theta=1/2$ and k=0.05 are the results produced by varying
the knots on each time line an improvement over the other
methods. The remaining results show that constant knot
spacing is superior. The practice of using a small time
step length to gain improvement in accuracy when varying
the knots on each time line (as observed in case study 2.2)
is not observed here. As previously explained in section 8.6,
this is because oscillations in the numerical solutions occur
close to the initial line and maximum errors always occur
on the second time line for each value of k used.

We now consider an overall view of the proposed methods by
initially examining computing time required in the evaluation
of the results. When the knots are fixed throughout time,
numerical solutions are obtained from the schemes (4.2.8)
or (4.3.1) depending on the problem concerned. Irrespective

of the knot partition used each of the schemes resulted

in a tri-diagonal system of equations which was solved

using an efficient numerical algorithm (see for example,

Mitchell and Griffiths (1980)) giving the required solutions.

Obtaining these solutions using either constant knot spacing,

or the knots of the local and global methods therefore requires

the same computer time. Using the IBM 370/135 machine

installed at Sheffield City Polytechnic this computing time

for hyperbolic equations was found to be 15.2 seconds. In

addition, the derivation of the knot partitions using the

local and global methods is a relatively simple procedure

requiring 2 seconds and 3.3 seconds of computer time,

respectively. When the technique of chapter 7 is employed

to obtain solutions by deriving different knot partitions

on each time line, then the amount of computation required

obviously increases. We have found that, to obtain numerical

solutions to hyperbolic equations using this procedure

requires 34.4 seconds of computer time. For parabolic

partial differential equations slightly less computing

time is required for each of the methods since the scheme

(4.3.1) employed is only two time level. The times required

are however comparable, with the technique in which knots

are chosen on each time line taking approximately twice as

long as the methods in which the knots are fixed throughout time.

In general, the results of the case studies suggest that when the solution of the partial differential equation is of symmetrical form for all time, then nothing is gained by varying the knots on each time line. However, in these cases the results show that improvement in accuracy over equally spaced knots is generally achieved by using either the local or global knot partitions and choosing the parameter θ to give equal weighting to each of the time lines. In addition, when the solution of the partial differential equation exhibits the form of a wave whose peak moves in the x direction as time progresses, then considerable benefit appears to be gained by varying the knots on each time line provided the step length k is chosen to be small. The algorithm for positioning the knots on each time line is automatic and does not require knowledge about the shape of the solution a priori. This technique may therefore be useful in obtaining solutions to other numerical problems. Two possible extensions are given in the following section.

9.2   Possible Extensions

(i)   Parabolic partial differential equations of the form

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2} + v \frac{\partial u}{\partial x} \quad , \tag{9.2.1}$$

where $D > 0$ and v are constants, are called "diffusion-convection" equations because of the physical processes they describe. Typically, u might be the concentration of a material which is convected with velocity v and diffusing according to the diffusion coefficient D. Particular interest has been focussed on problems in which the cell Peclet number P is given by

$$P = \frac{vh}{2D} \tag{9.2.2}$$

is large. In such situations spurious oscillations are introduced into finite difference solutions (see for example, Price, Cavendish and Varga (1968)) when the analytic solution is known to be non-oscillatory. Various methods have been proposed to overcome this problem, the most well-known being the technique of "upwinding" which has been used by Spalding (1972) in finite difference approximations and by Christie, Griffiths, Mitchell and Zienkiewicz (1976) in the use of finite elements. In the analysis of difference schemes Siemieniuch and Gladwell (1978) observed that solutions of (9.2.1) may be kept non-oscillatory by restricting the step

size h with respect to the coefficient v. However, for large values of v this is computationally expensive and a scheme which can restrict the step length h locally (in the region of the oscillations) may therefore be beneficial.

(ii) For moving boundary problems in heat flow the physical situation usually arises where an interface, or internal boundary, exists which moves as time progresses. The interface often takes the form shown in Figure 23 where region A contains a material in its solid form, region B the material in its liquid form and the boundary PQ varies due to melting or freezing of the material. If the position of the interface at time t is given by x=S(t) then, in one space dimension, a typical set of governing equations may be of the form (see for example, Meyer (1976))

$$\frac{\partial}{\partial x}\left[k_1(x,t)\ \frac{\partial u_1}{\partial x}\right]\ -\ c_1(x,t)\ \frac{\partial u_1}{\partial t} = F_1(x,t),\ o<x<S(t)$$

$$\frac{\partial}{\partial x}\left[k_2(x,t)\ \frac{\partial u_2}{\partial x}\right]\ -\ c_2(x,t)\ \frac{\partial u_2}{\partial t} = F_2(x,t),\ S(t)<x<1 \quad (9.2.3)$$

Specific conditions are assumed at the interface x=S(t), on the boundaries x=o and x=1 and on the initial line t=o. A summary of the numerical methods devised for the solution of

such "Stefan problems" is given in Ockendon and

Hodgkins (1975). In general, the solution is such that

significant changes in the solution may occur close to

the interface. A scheme in which knot points are optimally

chosen on each time line may therefore provide a suitable

method of solution.

TABLE 1

Internal knot positions used in Case Study 1.1

Local	Global	Transformation
0.117965	0.133776	0.223607
0.220349	0.234013	0.316228
0.316010	0.325845	0.387298
0.408487	0.413714	0.447214
0.500000	0.500000	0.500000
0.591513	0.586286	0.520000
0.683990	0.674155	0.580000
0.779651	0.765987	0.680000
0.882035	0.866224	0.820000

TABLE 2

Errors for Case Study 1.1 using k=0.05 for 10 time steps

	θ	Constant knot spacing $h = 0.1$	Variable knot spacing		
			Local	Global	Transformation
(a)	0	8.16×10^{-3}	7.46×10^{-3}	7.09×10^{-3}	Unstable
	1/4	3.25×10^{-3}	2.54×10^{-3}	2.10×10^{-3}	3.89×10^{-3}
	1/3	1.63×10^{-3}	9.08×10^{-4}	4.87×10^{-4}	2.25×10^{-3}
	1/2	1.64×10^{-3}	2.34×10^{-3}	2.73×10^{-3}	2.00×10^{-3}
	1	1.12×10^{-2}	1.19×10^{-2}	1.24×10^{-2}	1.10×10^{-2}
(b)	1/12	6.48×10^{-3}	5.81×10^{-3}	5.43×10^{-3}	Unstable
	(6.2.11)	1.11×10^{-5}	4.05×10^{-5}	1.26×10^{-4}	1.21×10^{-3}

TABLE 3

Errors for Case Study 1.1 using k=0.01 for 10 time steps

	θ	Constant knot spacing $h = 0.1$	Variable knot spacing		
			Local	Global	Transformation
(a)	0	4.71×10^{-4}	4.13×10^{-4}	3.76×10^{-4}	7.88×10^{-4}
	1/4	4.43×10^{-4}	3.63×10^{-4}	3.41×10^{-4}	7.78×10^{-4}
	1/3	3.95×10^{-4}	3.70×10^{-4}	3.32×10^{-4}	7.17×10^{-4}
	1/2	3.72×10^{-4}	3.42×10^{-4}	3.08×10^{-4}	7.37×10^{-4}
	1	3.80×10^{-4}	3.22×10^{-4}	2.96×10^{-4}	7.28×10^{-4}
(b)	(6.2.11)	4.39×10^{-5}	6.19×10^{-5}	2.04×10^{-5}	2.03×10^{-4}

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TABLE 4

Truncation Errors for Case Study 1.1 using k=0.05 for 10 time steps

θ	Constant knot spacing	Variable knot spacing		
	h = 0.1	Local	Global	Transformation
0	2.50×10^{-4}	1.87×10^{-4}	9.23×10^{-5}	Unstable
1/4	9.98×10^{-5}	7.34×10^{-5}	3.35×10^{-5}	2.36×10^{-2}
1/3	4.99×10^{-5}	3.55×10^{-5}	1.39×10^{-5}	5.03×10^{-2}
1/2	4.99×10^{-5}	5.27×10^{-5}	2.89×10^{-5}	1.04×10^{-1}
1	3.49×10^{-4}	2.68×10^{-4}	1.43×10^{-4}	2.65×10^{-1}

TABLE 5

Internal knot positions used in Case Study 1.2

Local	Global
0.104019	0.116725
0.228994	0.282605
0.397569	0.399465
0.501907	0.500314
0.595750	0.593166
0.683453	0.680781
0.766875	0.764549
0.847043	0.845305
0.924603	0.923605

TABLE 6

Errors for Case Study 1.2 using k=0.05 for 10 time steps

θ	Constant knot spacing $h = 0.1$	Variable knot spacing	
		Local	Global
(a) 0	1.10×10^{-2}	1.03×10^{-2}	9.35×10^{-3}
1/4	3.89×10^{-3}	2.32×10^{-3}	2.01×10^{-3}
1/3	2.28×10^{-3}	2.88×10^{-3}	2.84×10^{-3}
1/2	4.38×10^{-3}	6.93×10^{-3}	6.76×10^{-3}
1	1.21×10^{-2}	1.38×10^{-2}	1.36×10^{-2}
(b) (6.2.11)	2.61×10^{-3}	1.82×10^{-3}	1.92×10^{-3}

TABLE 7

Errors on second time line for Case Study 1.2

$$k = 0.05, \quad \theta = 1/3$$

Constant knot spacing h = 0.1	Variable knot spacing	
	Local	Global
1.01×10^{-3}	2.18×10^{-4}	2.65×10^{-4}

TABLE 8

Errors for Case Study 1.2 using k=0.01 for 10 time steps

θ	Constant knot spacing $h = 0.1$	Variable knot spacing Local	Global
0	3.22×10^{-3}	1.81×10^{-3}	1.86×10^{-3}
1/4	3.13×10^{-3}	1.71×10^{-3}	1.77×10^{-3}
1/3	3.10×10^{-3}	1.68×10^{-3}	1.74×10^{-3}
1/2	3.04×10^{-3}	1.62×10^{-3}	1.67×10^{-3}
1	2.86×10^{-3}	1.44×10^{-3}	1.50×10^{-3}

TABLE 9

Errors for Case Study 1.2 using k=0.01 for 50 time steps

θ	Constant knot spacing h = 0.1	Variable knot spacing Local	Global
0	1.00×10^{-2}	8.74×10^{-3}	8.76×10^{-3}
1/4	9.76×10^{-3}	8.24×10^{-3}	8.34×10^{-3}
1/3	9.65×10^{-3}	8.08×10^{-3}	8.20×10^{-3}
1/2	9.43×10^{-3}	7.72×10^{-3}	7.86×10^{-3}
1	8.83×10^{-3}	6.80×10^{-3}	7.03×10^{-3}

TABLE 10

Errors for Case Study 1.3 using $\theta = \frac{1}{3}$ and k=0.05 for 10 time steps

c	Constant knot spacing $h = 0.1$	Variable knot spacing	
		Local	Global
-1	5.58×10^{-4}	1.76×10^{-4}	5.19×10^{-4}
-10	7.54×10^{-3}	7.93×10^{-3}	8.15×10^{-3}
-100	1.52×10^{-1}	1.52×10^{-1}	1.53×10^{-1}
-200	2.93×10^{-1}	2.93×10^{-1}	2.93×10^{-1}

TABLE 11

Errors for Case Study 1.3 using $\theta = \frac{1}{3}$ and k=0.01 for 50 time steps

c	Constant knot spacing h = 0.1	Variable knot spacing	
		Local	Global
-1	6.29×10^{-3}	6.21×10^{-3}	5.55×10^{-3}
-10	4.11×10^{-3}	3.23×10^{-3}	3.16×10^{-3}
-100	4.58×10^{-3}	4.81×10^{-3}	4.94×10^{-3}
-200	1.41×10^{-2}	1.44×10^{-2}	1.45×10^{-2}

TABLE 12

Errors for Case Study 1.3 using $\theta=0$ and $k=0.05$ for 10 time steps

c	Constant knot spacing $h = 0.1$	Variable knot spacing Local	Global
-1	8.09×10^{-3}	7.43×10^{-3}	7.07×10^{-3}
-10	7.54×10^{-3}	7.17×10^{-3}	7.00×10^{-3}
-100	5.75×10^{-2}	5.72×10^{-2}	5.71×10^{-2}
-200	1.47×10^{-1}	1.47×10^{-1}	1.46×10^{-1}

TABLE 13

Errors for Case Study 1.4 using k=0.05 for 10 time steps

	θ	Constant knot spacing h = 0.1	Variable knot spacing Local	Global
(a)	1/4	Unstable	Unstable	Unstable
	1/2	1.08×10^{-2}	1.05×10^{-2}	1.03×10^{-2}
	3/4	3.39×10^{-2}	3.42×10^{-2}	3.44×10^{-2}
	1	7.32×10^{-2}	7.35×10^{-2}	7.37×10^{-2}
(b)	(6.4.5)	7.65×10^{-3}	7.63×10^{-3}	7.61×10^{-3}

TABLE 14

Errors for Case Study 1.4 using k=0.01 for 50 time steps

	θ	Constant knot spacing $h = 0.1$	Variable knot spacing Local	Global
(a)	1/4	Unstable	Unstable	Unstable
	1/2	3.33×10^{-3}	2.97×10^{-3}	2.77×10^{-3}
	3/4	5.72×10^{-3}	6.07×10^{-3}	6.27×10^{-3}
	1	1.46×10^{-2}	1.49×10^{-2}	1.51×10^{-2}
(b)	(6.4.5)	2.87×10^{-4}	2.71×10^{-4}	2.48×10^{-4}

TABLE 15

Internal knot positions used in Case Study 1.5 when a=1.

Local	Global
0.089594	0.089472
0.181218	0.180988
0.274965	0.274652
0.370935	0.370557
0.469235	0.468818
0.569981	0.569558
0.673296	0.672893
0.779315	0.778977
0.888182	0.887945

TABLE 16

Internal knot positions used in Case Study 1.5 when a=10

Local	Global
0.041330	0.038513
0.087159	0.081132
0.138550	0.128841
0.196988	0.183019
0.264618	0.245703
0.344707	0.320070
0.442549	0.411493
0.567504	0.530205
0.738279	0.699769

TABLE 17

Errors for Case Study 1.5 when a=1 and k=0.05

	θ	Constant knot spacing h = 0.1	Variable knot spacing Local	Global
(a)	1/4	Unstable	Unstable	Unstable
	1/2	3.00×10^{-3}	2.89×10^{-3}	2.89×10^{-3}
	3/4	2.73×10^{-3}	2.74×10^{-3}	2.74×10^{-3}
	1	5.77×10^{-3}	5.83×10^{-3}	5.83×10^{-3}
(b)	(6.4.5)	2.72×10^{-3}	2.67×10^{-3}	2.67×10^{-3}

TABLE 18

Errors for Case Study 1.5 when a=1 and k=0.01

θ	Constant knot spacing $h = 0.1$	Variable knot spacing	
		Local	Global
(a) 1/4	Unstable	Unstable	Unstable
1/2	7.04×10^{-4}	6.99×10^{-4}	6.99×10^{-4}
3/4	4.63×10^{-4}	4.73×10^{-4}	4.72×10^{-4}
1	1.17×10^{-3}	1.18×10^{-3}	1.18×10^{-3}
(b) (6.4.5)	3.92×10^{-4}	4.36×10^{-4}	4.37×10^{-4}

TABLE 19

Errors for Case Study 1.5 when a = 10 and k = 0.05

θ	Constant knot spacing $h = 0.1$	Variable knot spacing Loacl	Global
(a) 1/4	Unstable	Unstable	Unstable
1/2	1.55×10^{-1}	1.48×10^{-1}	1.48×10^{-1}
3/4	3.54×10^{-2}	3.72×10^{-2}	3.84×10^{-2}
1	8.01×10^{-2}	8.32×10^{-2}	8.29×10^{-2}
(b) (6.4.5)	1.43×10^{-1}	1.45×10^{-1}	1.45×10^{-1}

Table 20

Errors for Case Study 1.5 when a = 10 and k = 0.01

	θ	Constant knot spacing $h = 0.1$	Variable knot spacing Local	Global
(a)	1/4	Unstable	Unstable	Unstable
	1/2	4.49×10^{-2}	4.86×10^{-2}	4.77×10^{-2}
	3/4	1.09×10^{-2}	1.76×10^{-2}	1.73×10^{-3}
	1	3.29×10^{-2}	3.95×10^{-2}	3.93×10^{-2}
(b)	(6.4.5)	2.68×10^{-2}	4.47×10^{-2}	4.43×10^{-2}

TABLE 21

Errors for Case Study 2.1 using k=0.05 for 10 time steps

θ	Constant knot spacing h=0-1	Variable knot spacing		Varying the knots on each time line
		Local	Global	
0	8.16×10^{-3}	7.46×10^{-3}	7.09×10^{-3}	7.34×10^{-3}
1/4	3.25×10^{-3}	2.54×10^{-3}	2.10×10^{-3}	2.39×10^{-3}
1/3	1.63×10^{-3}	9.08×10^{-4}	4.87×10^{-4}	7.61×10^{-4}
1/2	1.64×10^{-3}	2.34×10^{-3}	2.73×10^{-3}	2.48×10^{-3}
1	1.12×10^{-2}	1.19×10^{-2}	1.24×10^{-2}	1.21×10^{-2}

<center>TABLE 22</center>

Errors for Case Study 2.2 using k=0.05 for 10 time steps

θ	Constant knot spacing h=0.1	Variable knot spacing Local	Global	Varying the knots on each time line
0	1.10×10^{-2}	1.03×10^{-2}	9.35×10^{-3}	2.17×10^{-2}
1/4	3.89×10^{-3}	2.32×10^{-3}	2.01×10^{-3}	3.48×10^{-3}
1/3	2.28×10^{-3}	2.88×10^{-3}	2.84×10^{-3}	4.17×10^{-3}
1/2	4.38×10^{-3}	6.93×10^{-3}	6.76×10^{-3}	9.85×10^{-3}
1	1.21×10^{-2}	1.38×10^{-2}	1.36×10^{-2}	1.55×10^{-2}

TABLE 23

Errors for Case Study 2.2 using k=0.01 for 50 time steps

θ	Constant knot spacing $h=0.1$	Variable knot spacing Local	Global	Varying the knots on each time line
0	1.00×10^{-2}	8.74×10^{-3}	8.76×10^{-3}	4.48×10^{-3}
1/4	9.76×10^{-3}	8.24×10^{-3}	8.34×10^{-3}	5.07×10^{-3}
1/3	9.65×10^{-3}	8.08×10^{-3}	8.20×10^{-3}	5.21×10^{-3}
1/2	9.43×10^{-3}	7.72×10^{-3}	7.86×10^{-3}	4.60×10^{-3}
1	8.83×10^{-3}	6.80×10^{-3}	7.03×10^{-3}	5.02×10^{-3}

TABLE 24

Errors for Case Study 2.3 using $\theta = \frac{1}{3}$ and k=0.05 for 10 time steps

c	Constant knot spacing h=0.1	Variable knot spacing Local	Global	Varying the knots on each time line
-1	5.58×10^{-4}	1.76×10^{-4}	5.19×10^{-4}	3.22×10^{-4}
-10	7.54×10^{-3}	7.93×10^{-3}	8.15×10^{-3}	8.04×10^{-3}
-100	1.52×10^{-1}	1.52×10^{-1}	1.53×10^{-1}	1.52×10^{-1}
-200	2.93×10^{-1}	2.93×10^{-1}	2.93×10^{-1}	2.93×10^{-1}

TABLE 25

Errors for Case Study 2.3 using $\theta = \frac{1}{3}$ and k=0.01 for 50 time steps

c	Constant knot spacing h=0.1	Variable knot spacing		Varying the knots on each time line
		Local	Global	
-1	6.29×10^{-3}	6.21×10^{-3}	5.55×10^{-3}	5.90×10^{-3}
-10	4.11×10^{-3}	3.23×10^{-3}	3.16×10^{-3}	3.27×10^{-3}
-100	4.58×10^{-3}	4.81×10^{-3}	4.94×10^{-3}	4.92×10^{-3}
-200	1.41×10^{-2}	1.44×10^{-2}	1.45×10^{-2}	1.43×10^{-2}

TABLE 26

Errors for Case Study 2.4 using k=0.05 for 10 time steps

θ	Constant knot spacing h=0.1	Variable knot spacing Local	Global	Varying the knots on each time line
1/2	1.08×10^{-2}	1.05×10^{-2}	1.03×10^{-2}	1.04×10^{-2}
3/4	3.39×10^{-2}	3.42×10^{-2}	3.44×10^{-2}	3.43×10^{-2}
1	7.32×10^{-2}	7.35×10^{-2}	7.37×10^{-2}	7.35×10^{-2}

TABLE 27

Errors for Case Study 2.4 using k=0.01 for 50 time steps

θ	Constant knot spacing h=0.1	Variable knot spacing		Varying the knots on each time line
		Local	Global	
1/2	3.33×10^{-3}	2.97×10^{-3}	2.77×10^{-3}	2.90×10^{-3}
3/4	5.72×10^{-3}	6.07×10^{-3}	6.27×10^{-3}	6.14×10^{-3}
1	1.46×10^{-2}	1.49×10^{-2}	1.51×10^{-2}	1.50×10^{-2}

TABLE 28

Errors for Case Study 2.5 when a=1 and k=0.05

θ	Constant knot spacing h=0.1	Variable knot spacing Local	Global	Varying the knots on each-time line
1/4	Unstable	Unstable	Unstable	Unstable
1/2	3.00×10^{-3}	2.89×10^{-3}	2.89×10^{-3}	2.86×10^{-3}
3/4	2.73×10^{-3}	2.74×10^{-3}	2.74×10^{-3}	2.71×10^{-3}
1	5.77×10^{-3}	5.83×10^{-3}	5.83×10^{-3}	5.84×10^{-3}

TABLE 29

Errors for Case Study 2.5 when a=1 and k=0.01

θ	Constant knot spacing h=0.1	Variable knot spacing Local	Global	Varying the knots on each time line
1/4	Unstable	Unstable	Unstable	Unstable
1/2	7.04×10^{-4}	6.99×10^{-4}	6.99×10^{-4}	6.81×10^{-4}
3/4	4.63×10^{-4}	4.73×10^{-4}	4.72×10^{-4}	5.01×10^{-4}
1	1.17×10^{-3}	1.18×10^{-3}	1.18×10^{-3}	1.20×10^{-3}

TABLE 30

Errors for Case Study 2.5 when a=10 and k=0.05

θ	Constant knot spacing h=0.1	Variable knot spacing Local	Global	Varying the knots on each time line
1/4	Unstable	Unstable	Unstable	Unstable
1/2	1.55×10^{-1}	1.48×10^{-1}	1.48×10^{-1}	1.45×10^{-1}
3/4	3.54×10^{-2}	3.72×10^{-2}	3.84×10^{-2}	3.67×10^{-2}
1	8.01×10^{-2}	8.32×10^{-2}	8.29×10^{-2}	8.19×10^{-2}

TABLE 31

Errors for Case Study 2.5 when a=10 and k=0.01

θ	Constant knot spacing h=0.1	Variable knot spacing Local	Global	Varying the knots on each time line
1/4	unstable	Unstable	Unstable	Unstable
1/2	4.49×10^{-2}	4.86×10^{-2}	4.77×10^{-2}	5.01×10^{-2}
3/4	1.09×10^{-2}	1.76×10^{-2}	1.73×10^{-2}	1.45×10^{-2}
1	3.29×10^{-2}	3.95×10^{-2}	3.93×10^{-2}	4.02×10^{-2}
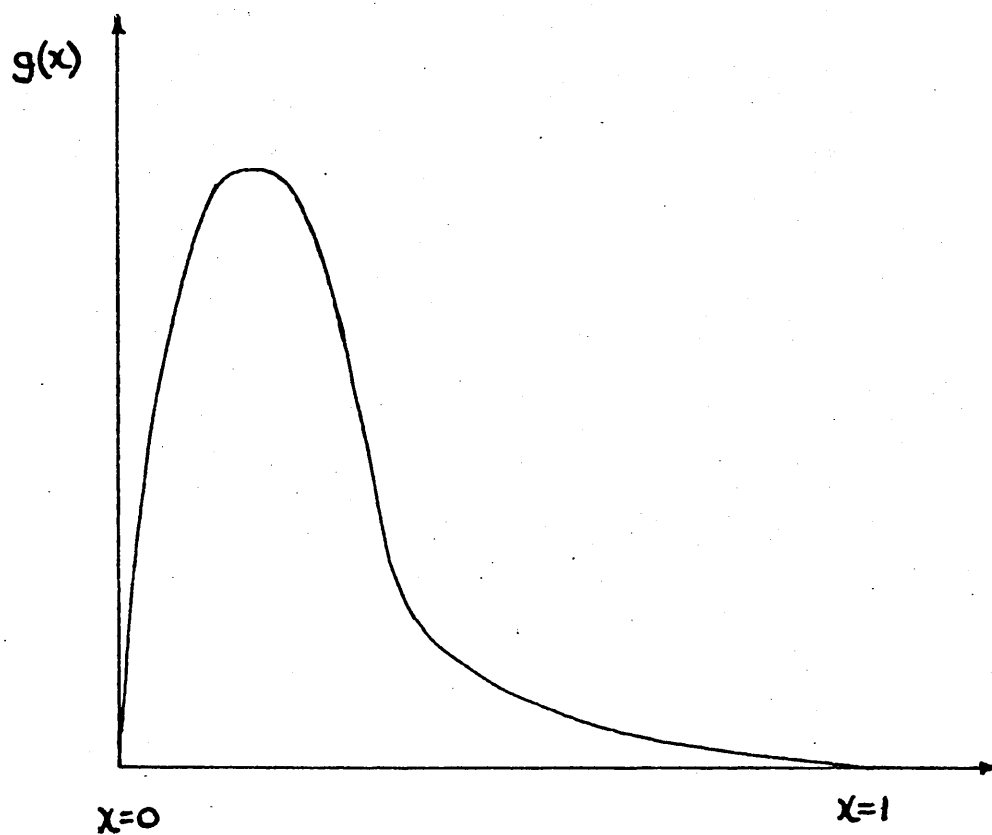
Figure 1

Shape of initial condition u(x,o)=g(x)

142
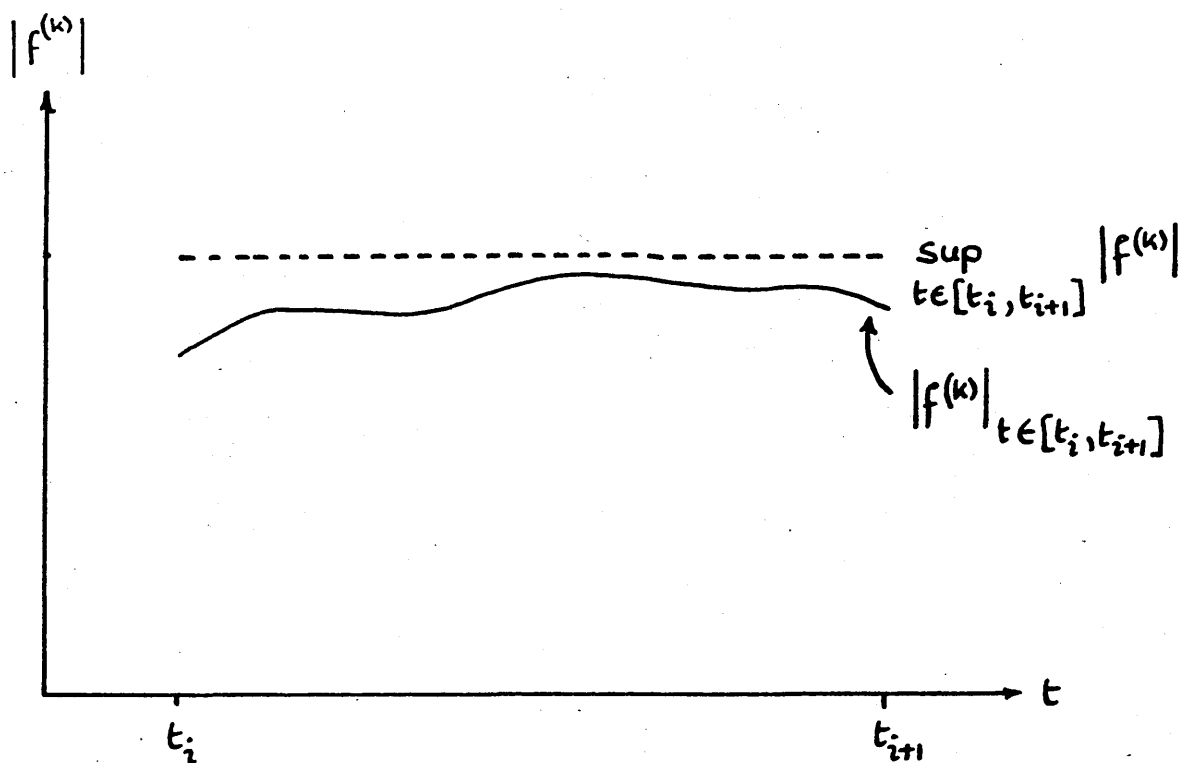
Figure 2(a)

Illustration of $\left\| f^{(k)} \right\|_i$
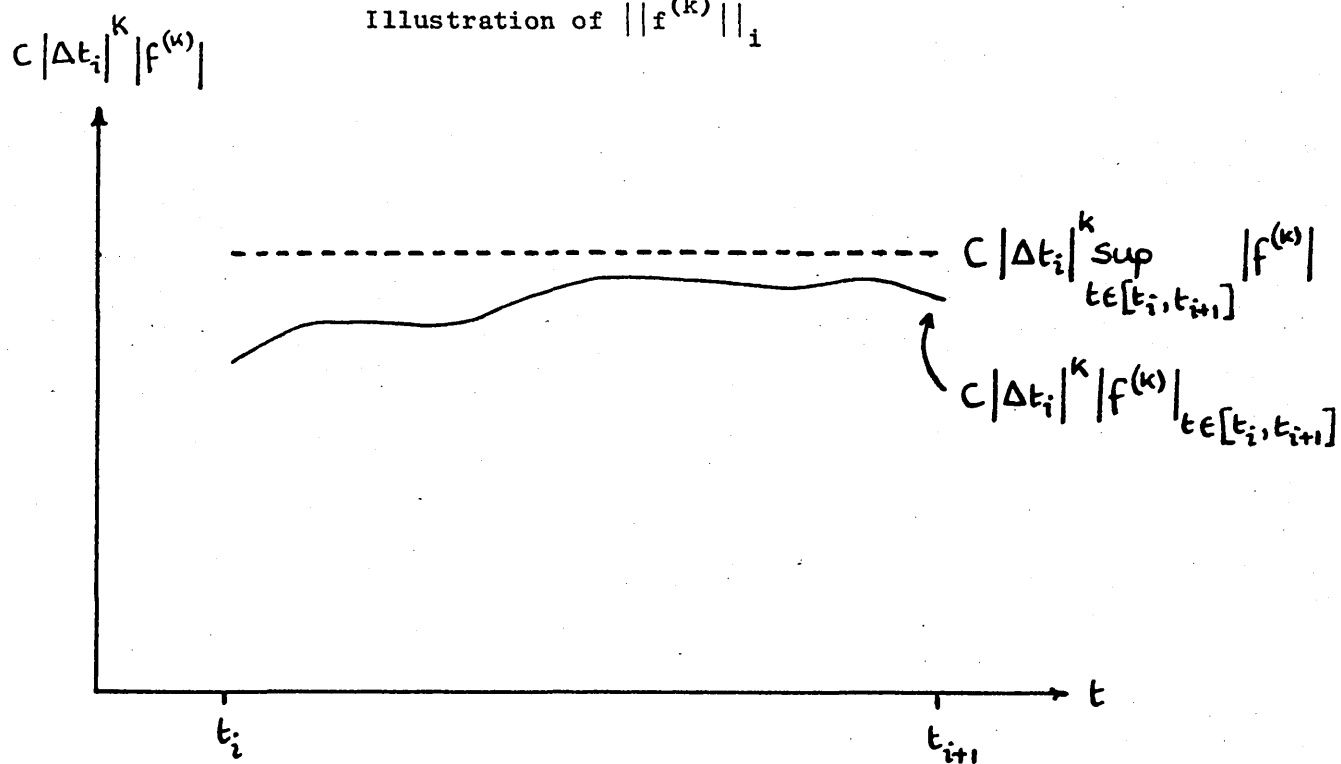
Figure 2(b)

Illustration of (5.3.2)
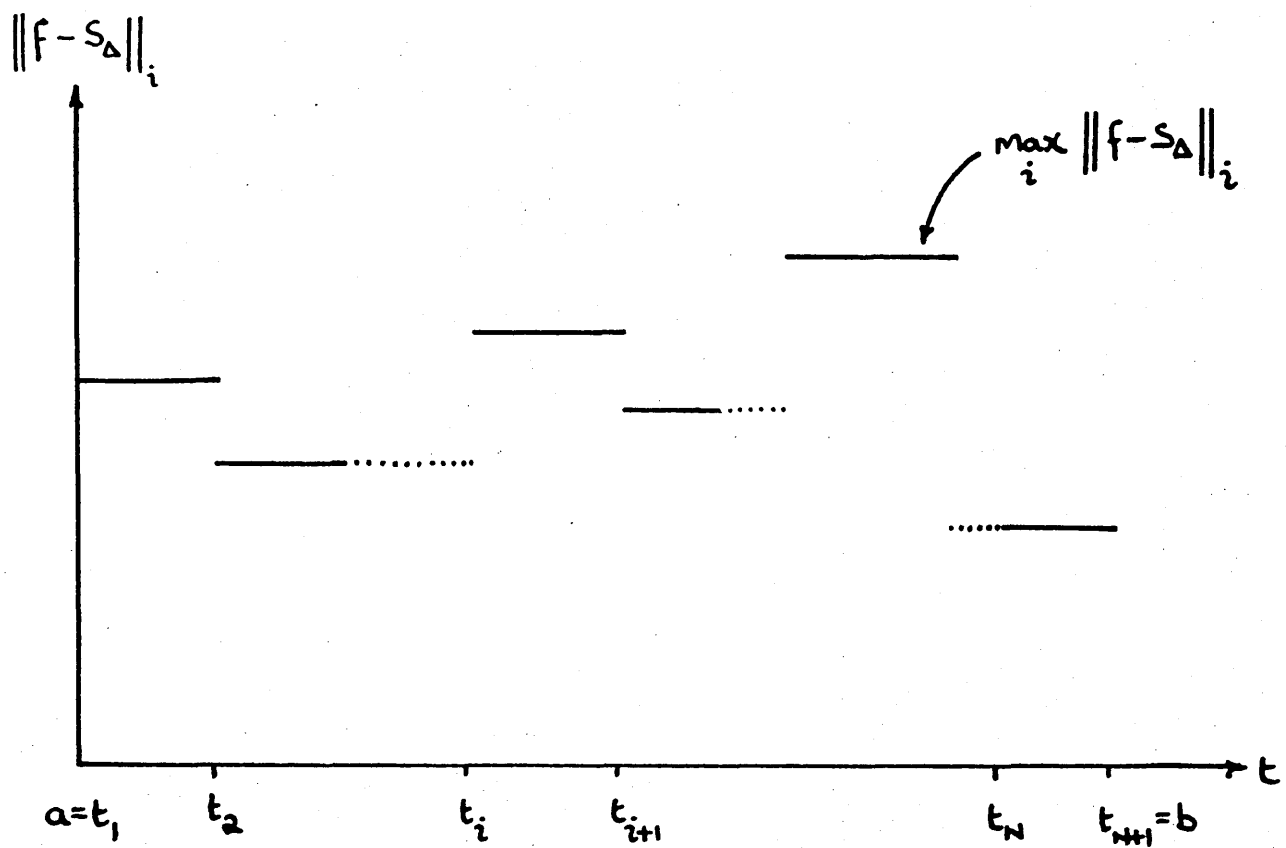
Figure 3

Illustration of $||f - s_\Delta||_\infty$

144
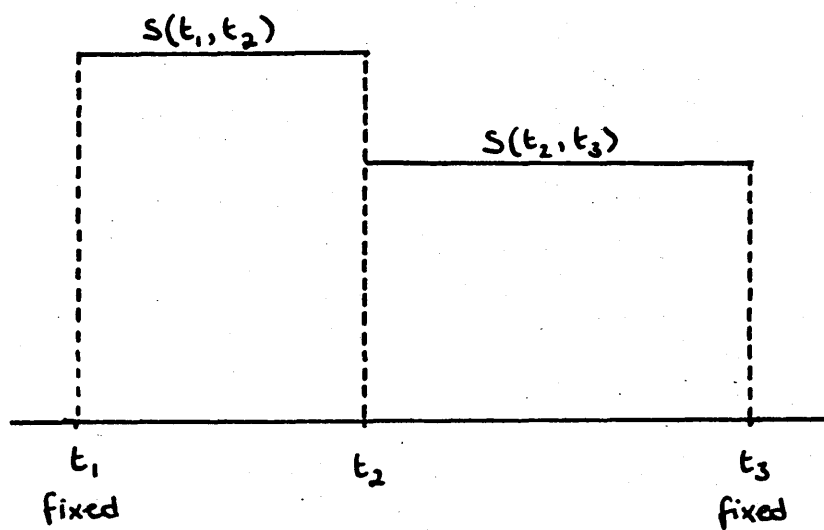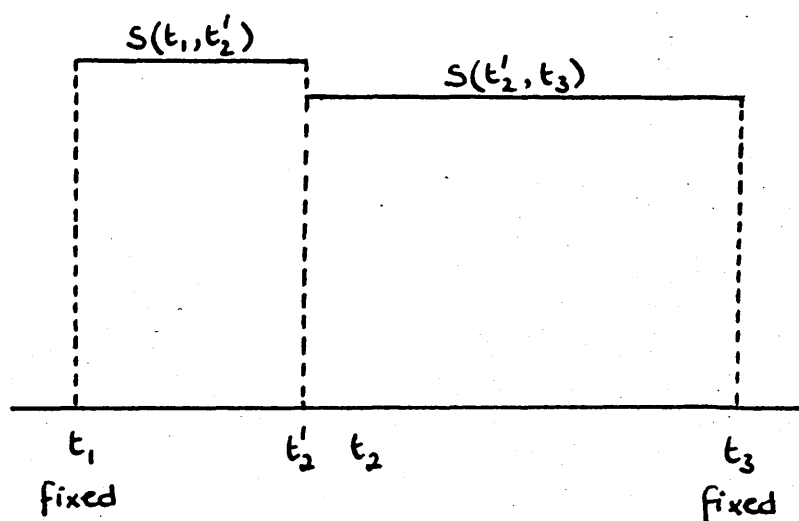
Figure 4(a)

Figure 4(b)

Locating the knot point t_2 – Global Method
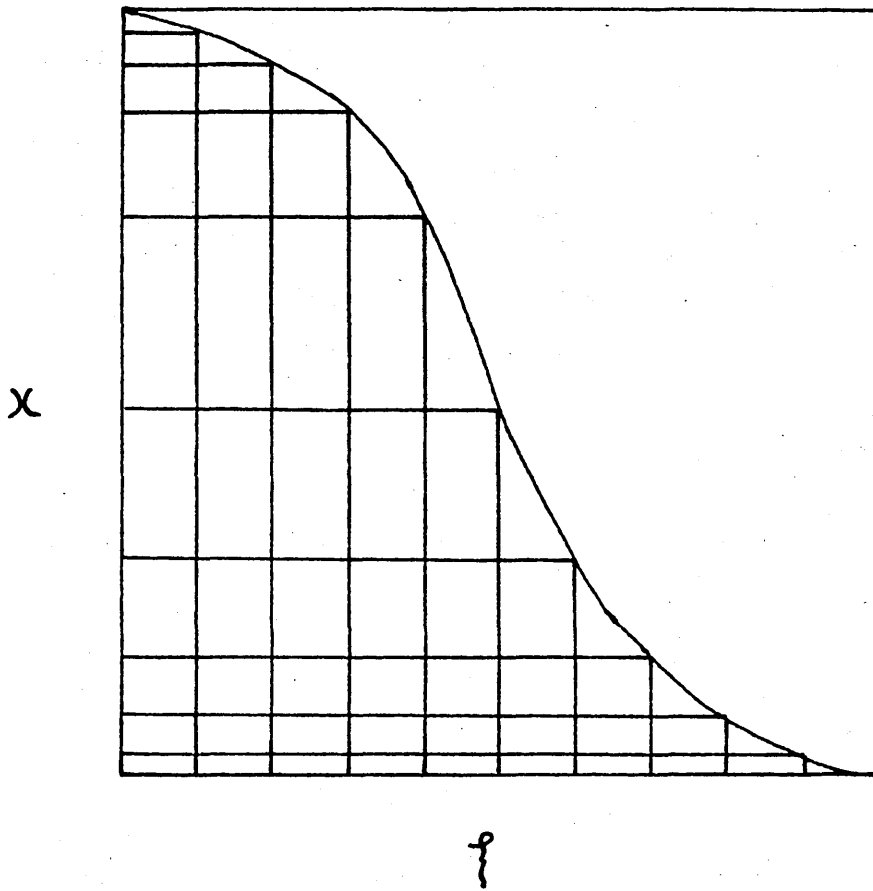
Figure 5

A transformation from a uniform mesh ξ to a non-uniform mesh x.

146
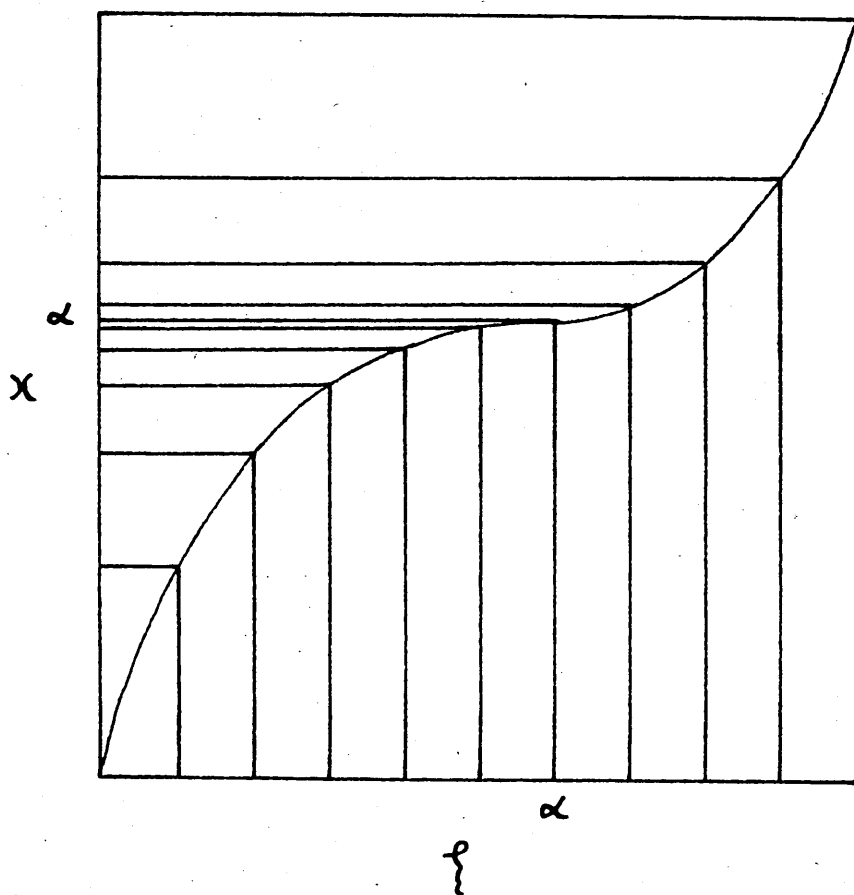
Figure 6

Transformation for a peak at x=α.
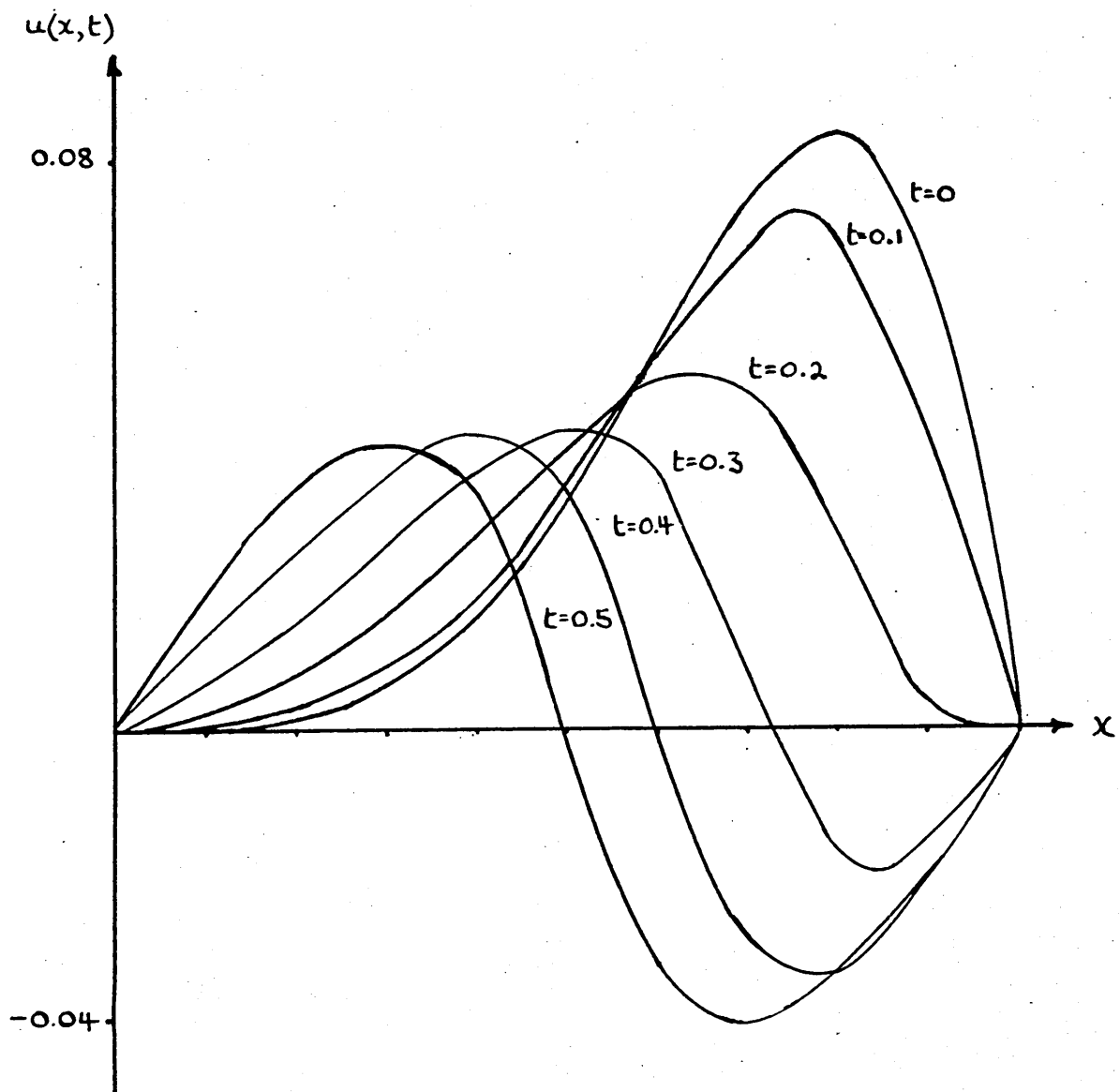
Figure 7

Shape of Analytic Solution (6.3.6) as time progresses

148
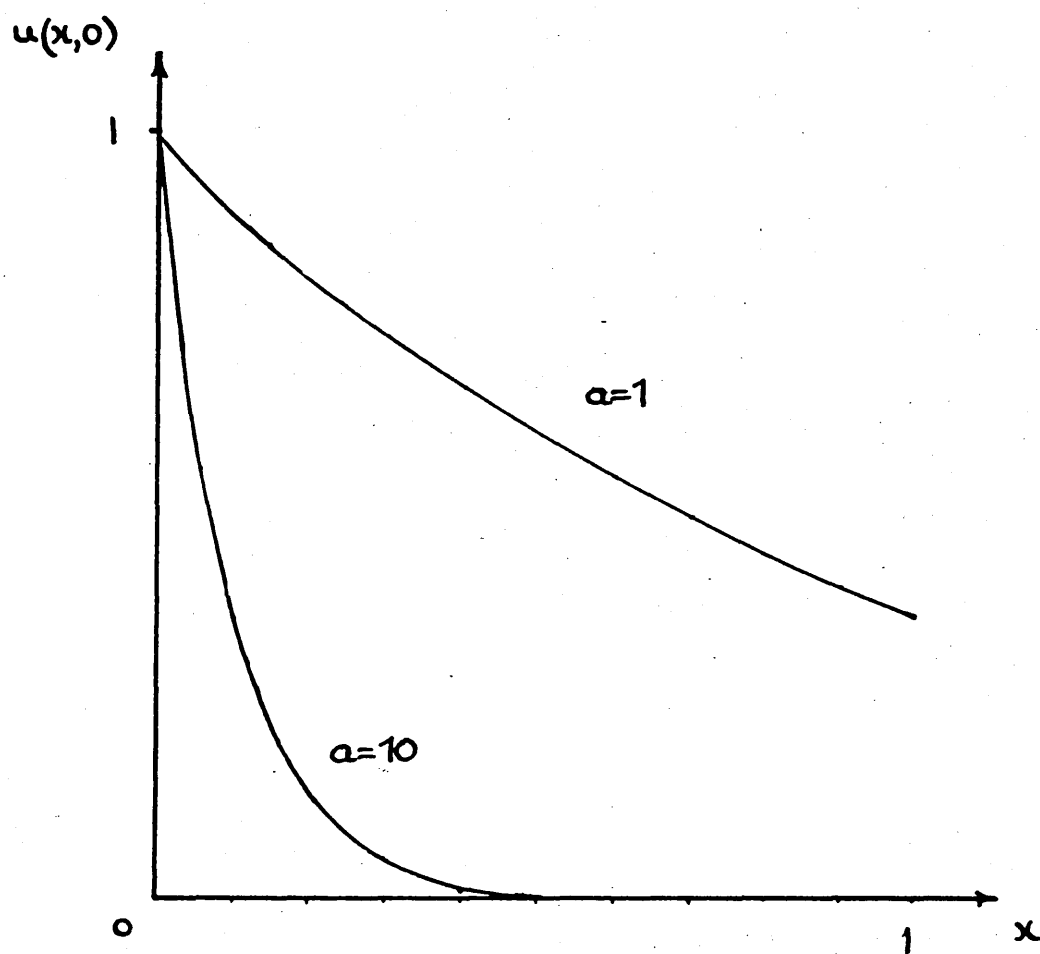
Figure 8

Shape of initial conditions used in Case Study 4

149
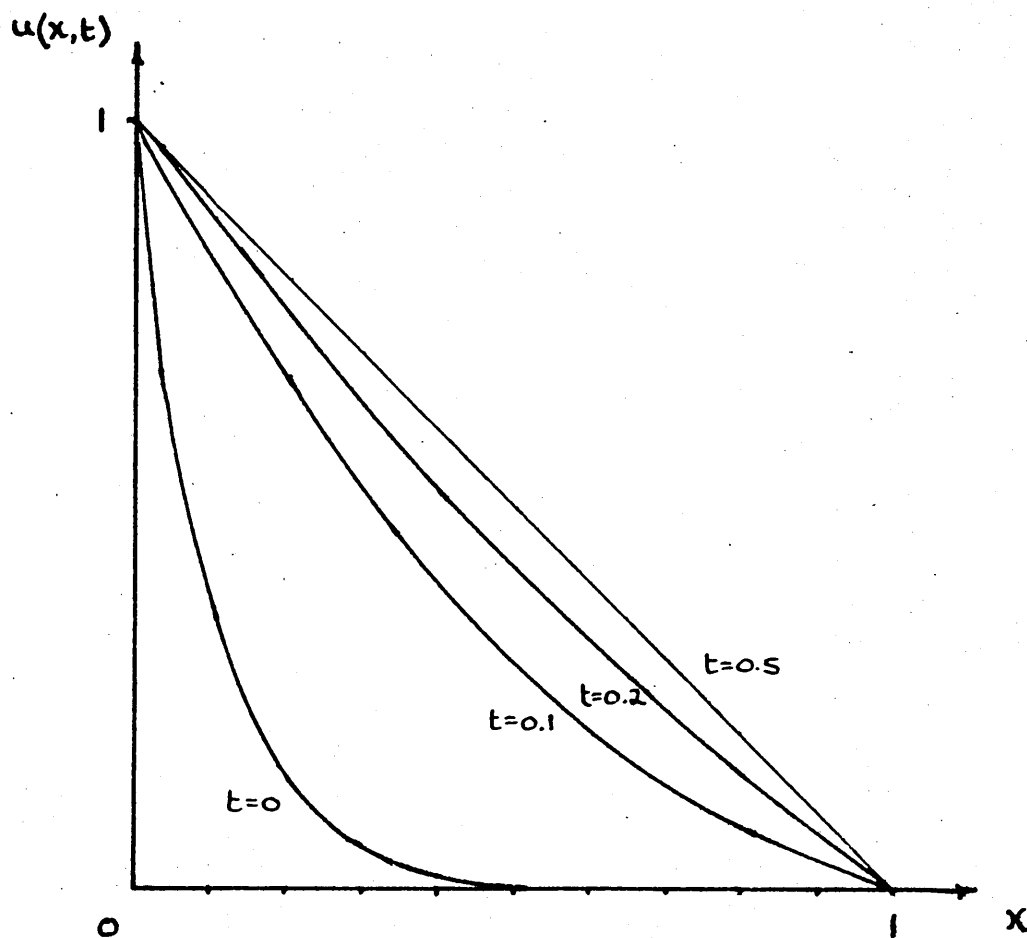
Figure 9

Shape of Analytic Solution (6.5.6),for various time

lines, using a=10.
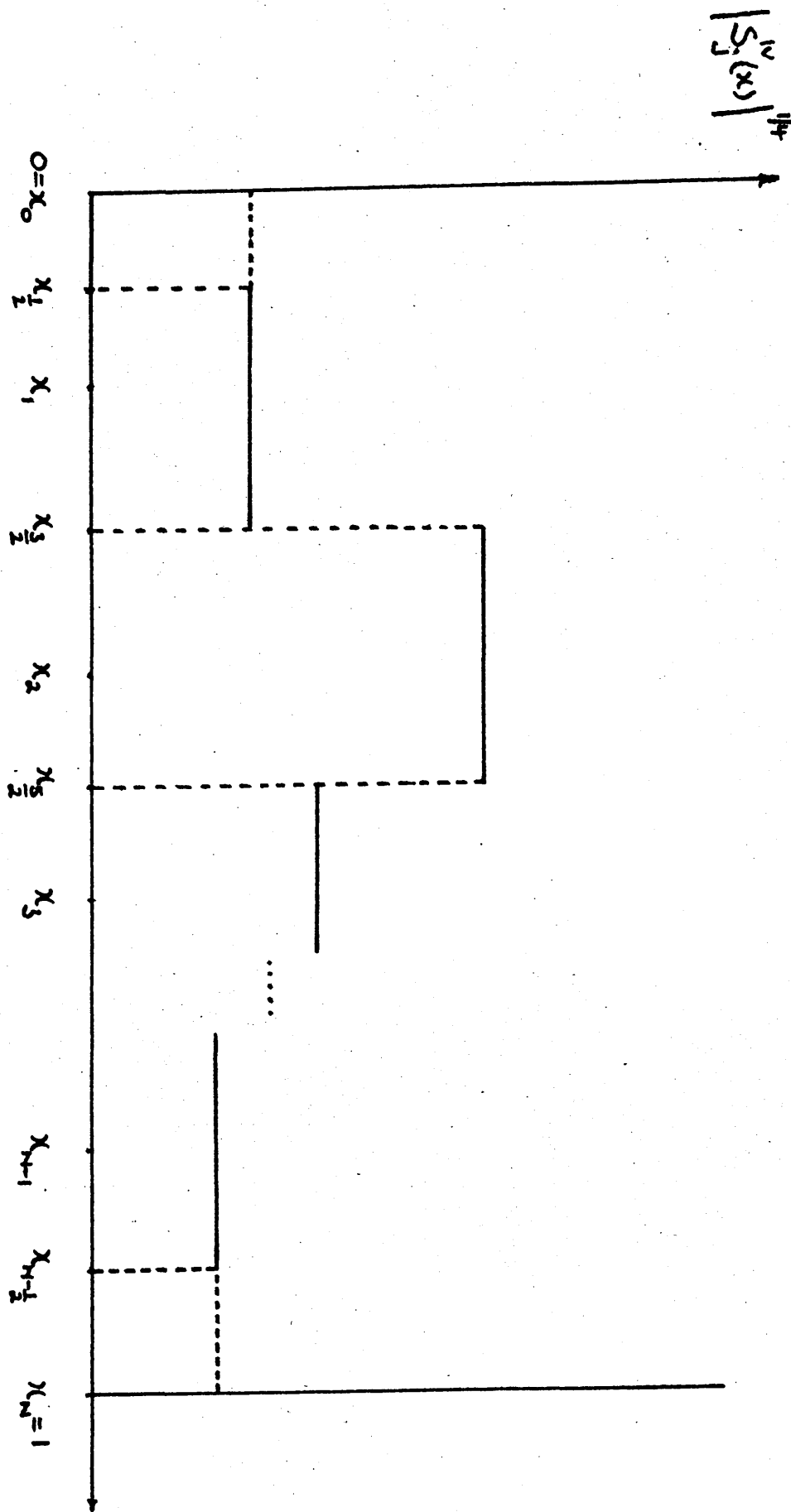
Figure 10

Illustration of (7.2.4)

151
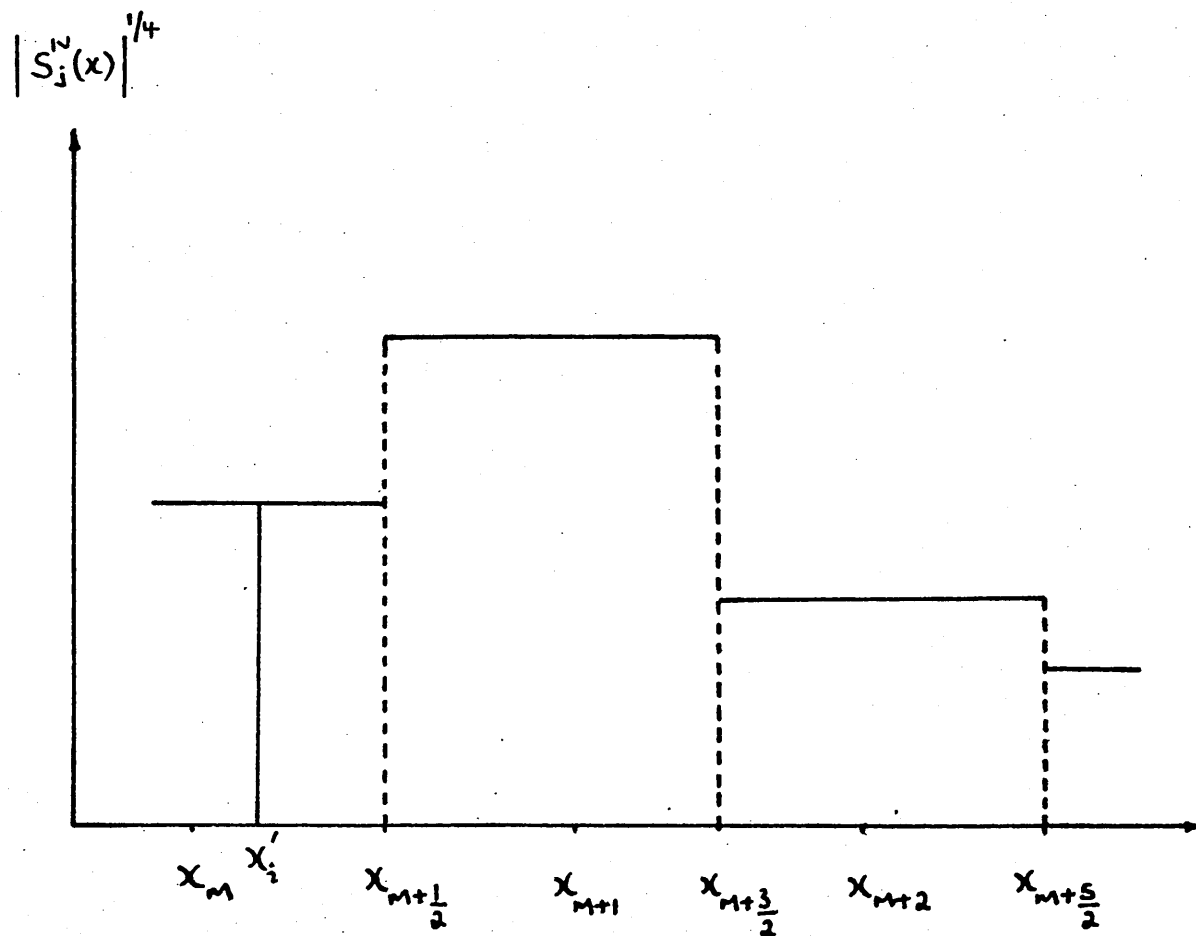
Figure 11

Illustration of procedure for determining new knots

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Π_{10} $t=0.5$

Π_8 $t=0.4$

Π_6 $t=0.3$

Π_4 $t=0.2$

Π_2 $t=0.1$

Π_0 $t=0$

$\chi=0$ $\chi=1$
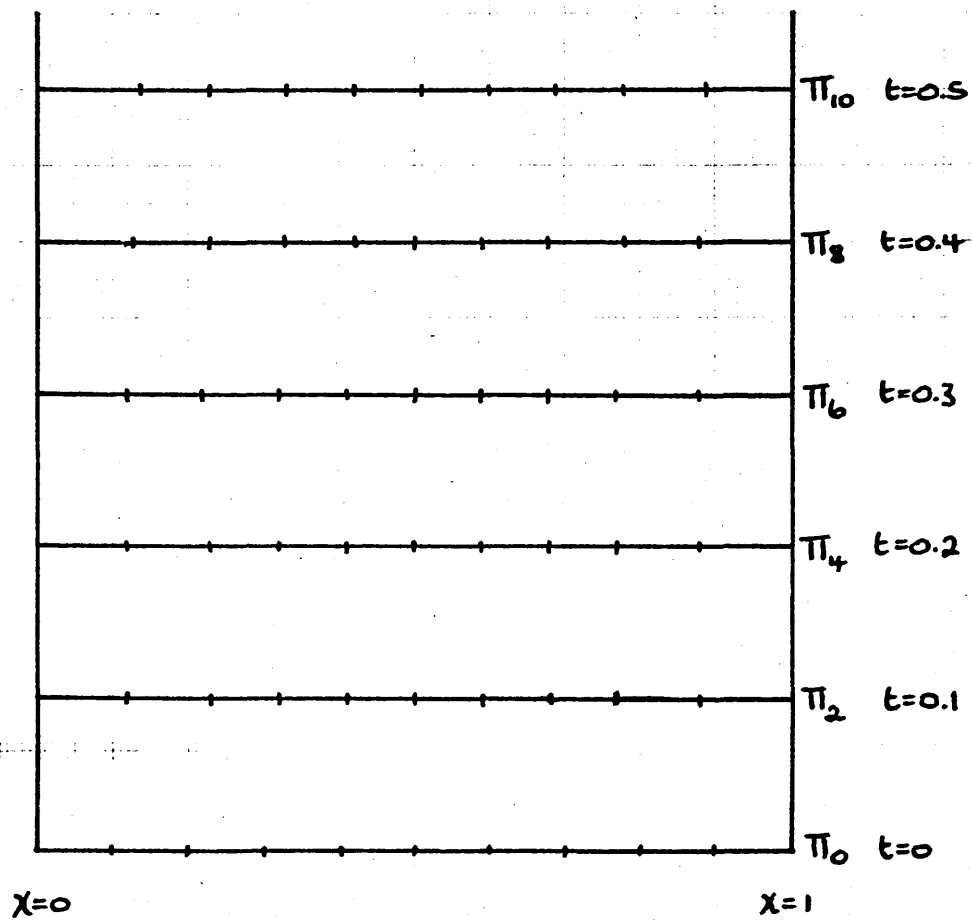
Figure 12

Knot Partitions for Case Study 2.1 with $\theta = \frac{1}{3}$, k=0.05
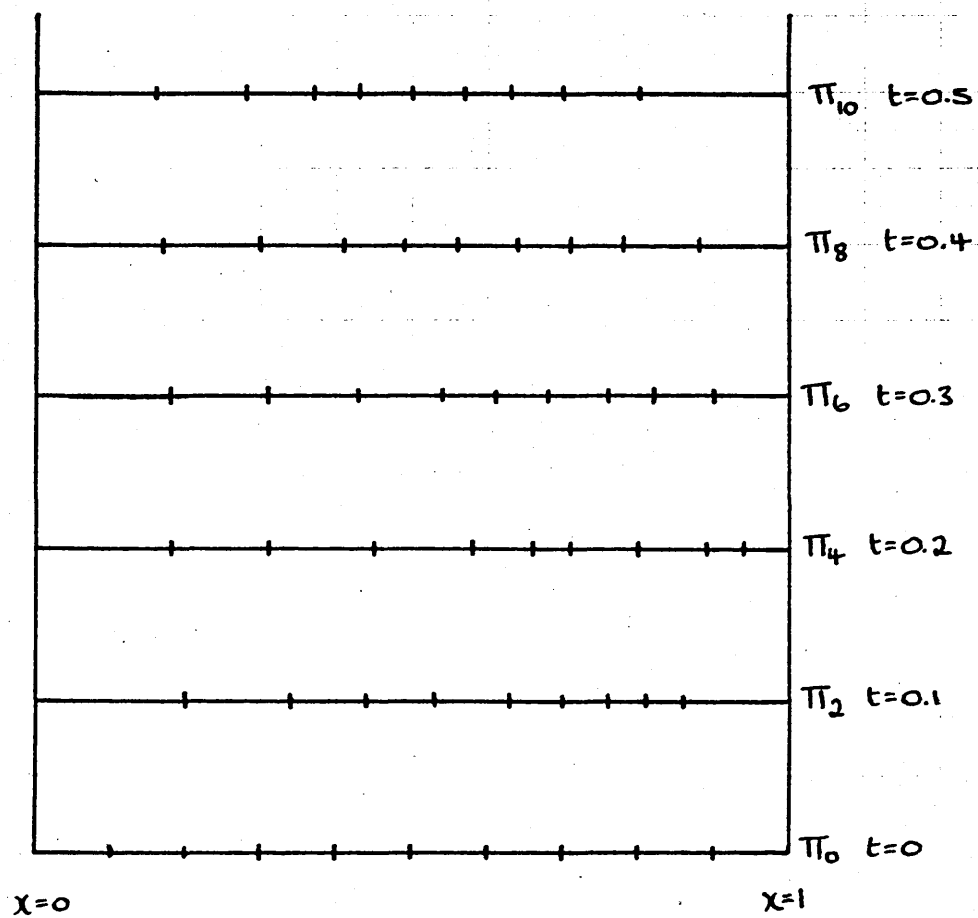
Figure 13

Knot Partitions for Case Study 2.2 with $\theta = \frac{1}{3}$ and k=0.05
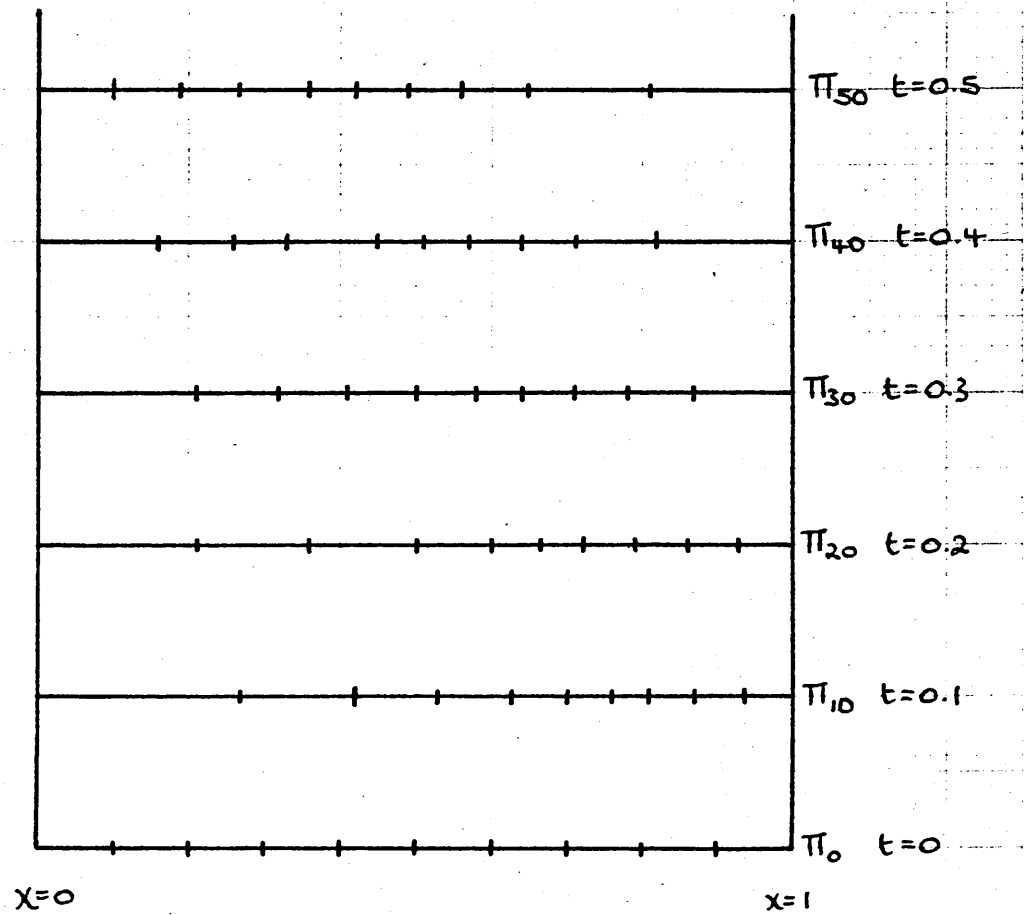
Figure 14

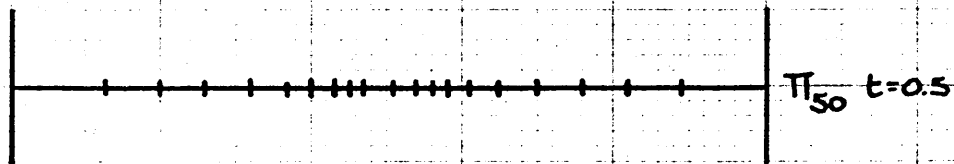Knot Partitions for Case Study 2.2 with $\theta = \frac{1}{3}$ and k=0.01
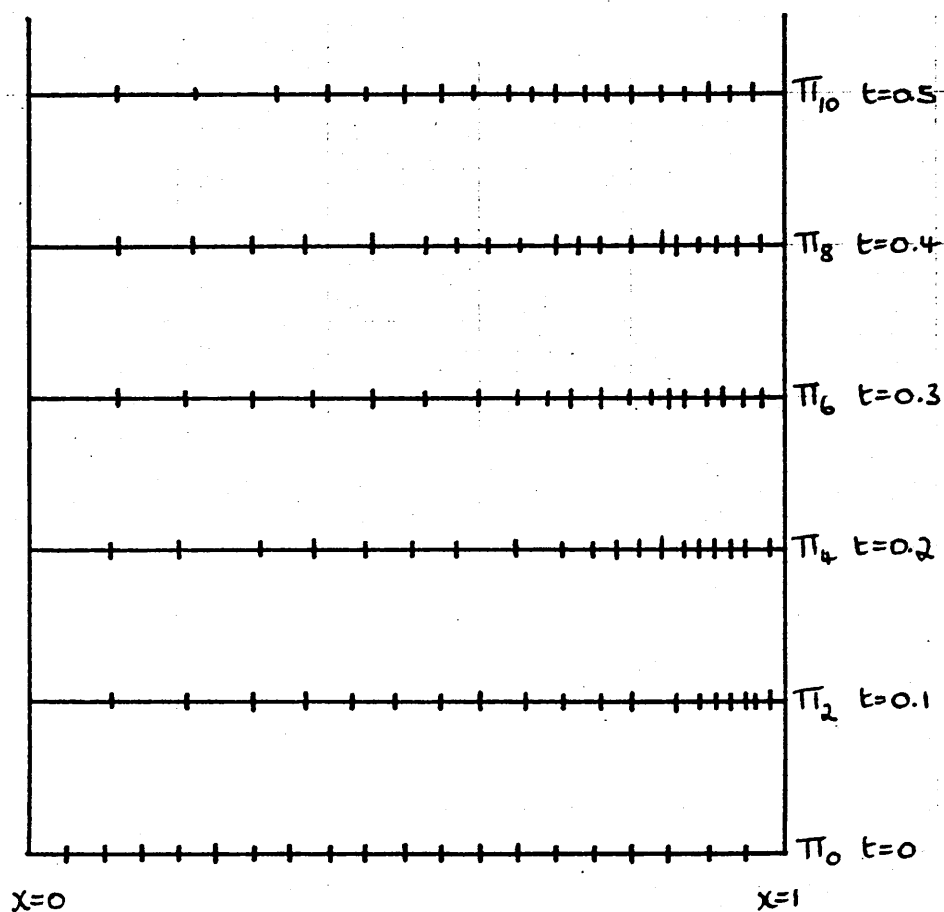
Figure 15

Knot Partitions for Case Study 2.2 with $\theta = \frac{1}{3}$ and k=0.05
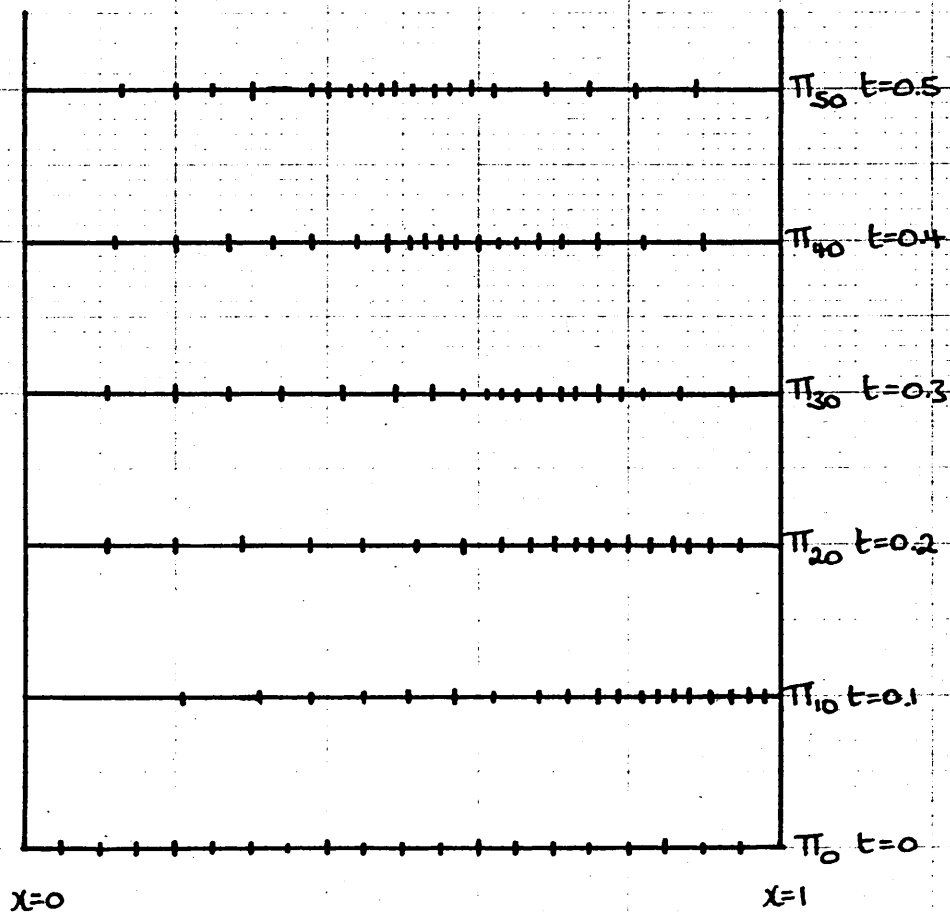
Figure 16

Knot Partitions for Case Study 2.2 with $\theta = \dfrac{1}{3}$ and k=0.01

Figure 17

Knot Partitions for Case STudy 2.2 using
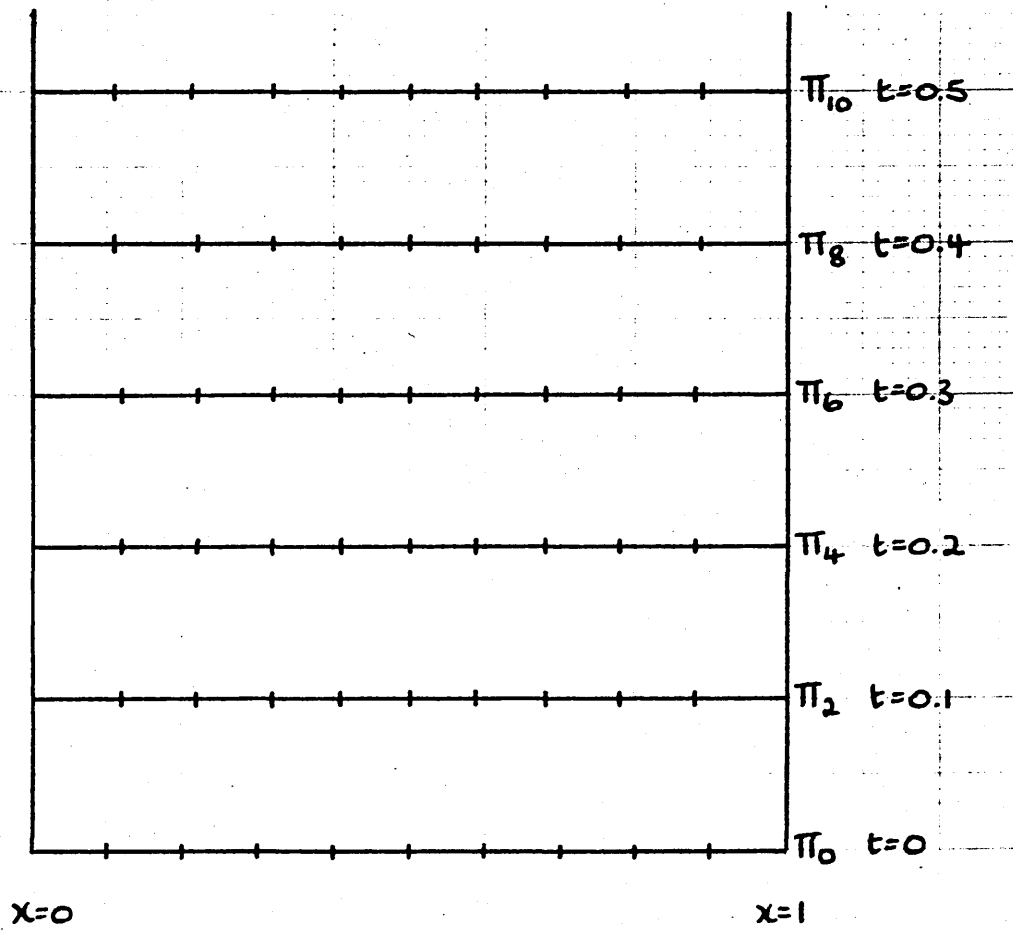the Analytic Solution (6.3.6) with k=0.01

Π_{10} t=0.5

Π_8 t=0.4

Π_6 t=0.3

Π_4 t=0.2

Π_2 t=0.1

Π_0 t=0

X=0

X=1

Figure 18

Knot Partitions for Case Study 2.4 with $\theta = \dfrac{1}{2}$ and k=0.05

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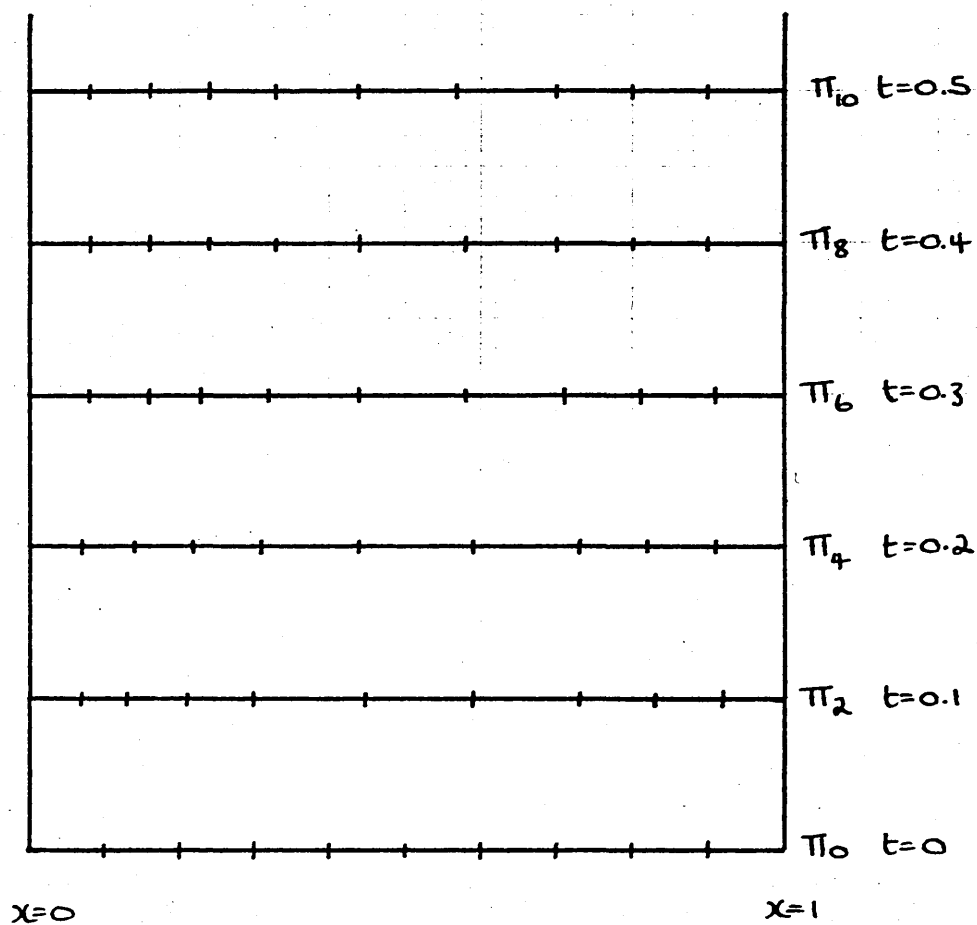
Figure 19

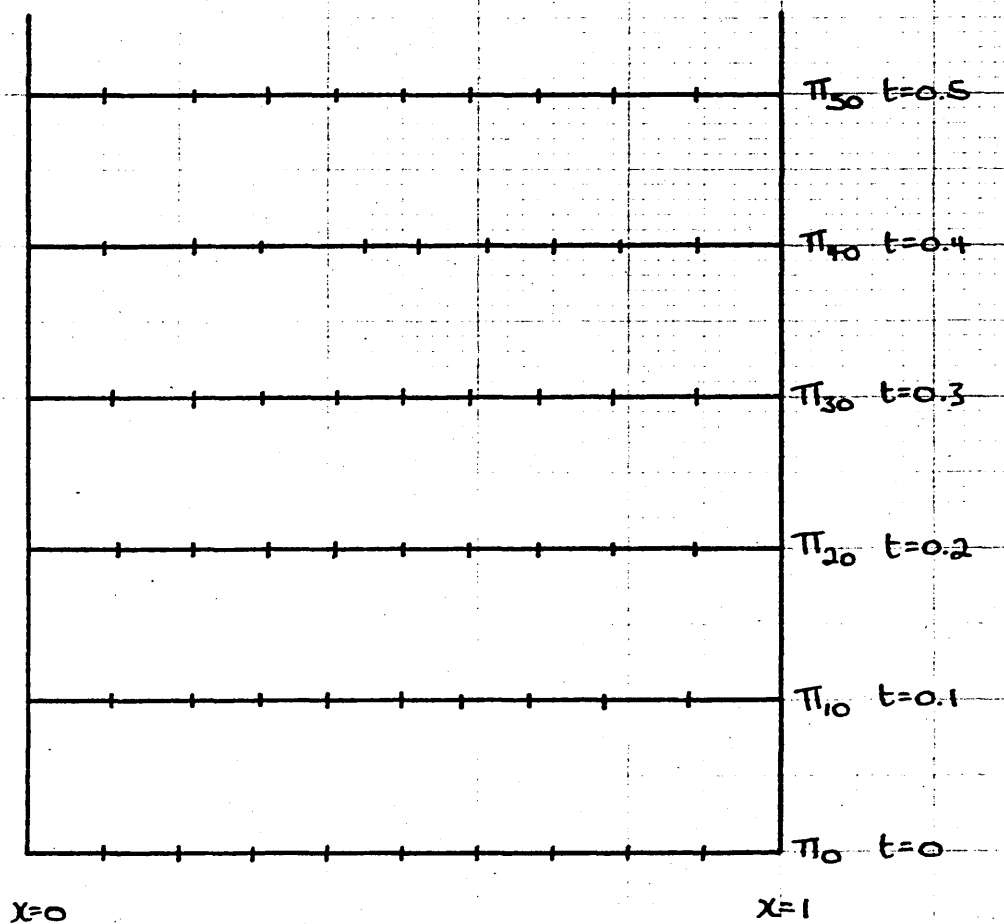Knot Partitions for Case Study 2.5 with a=1, k=0.05, $\theta = \frac{1}{2}$.

Figure 20

Knot Partitions for Case Study 2.5 with a=1, k=0.01, $\theta = \frac{1}{2}$.

Π_{10} t=0.5

Π_{8} t=0.4

Π_{6} t=0.3

Π_{4} t=0.2

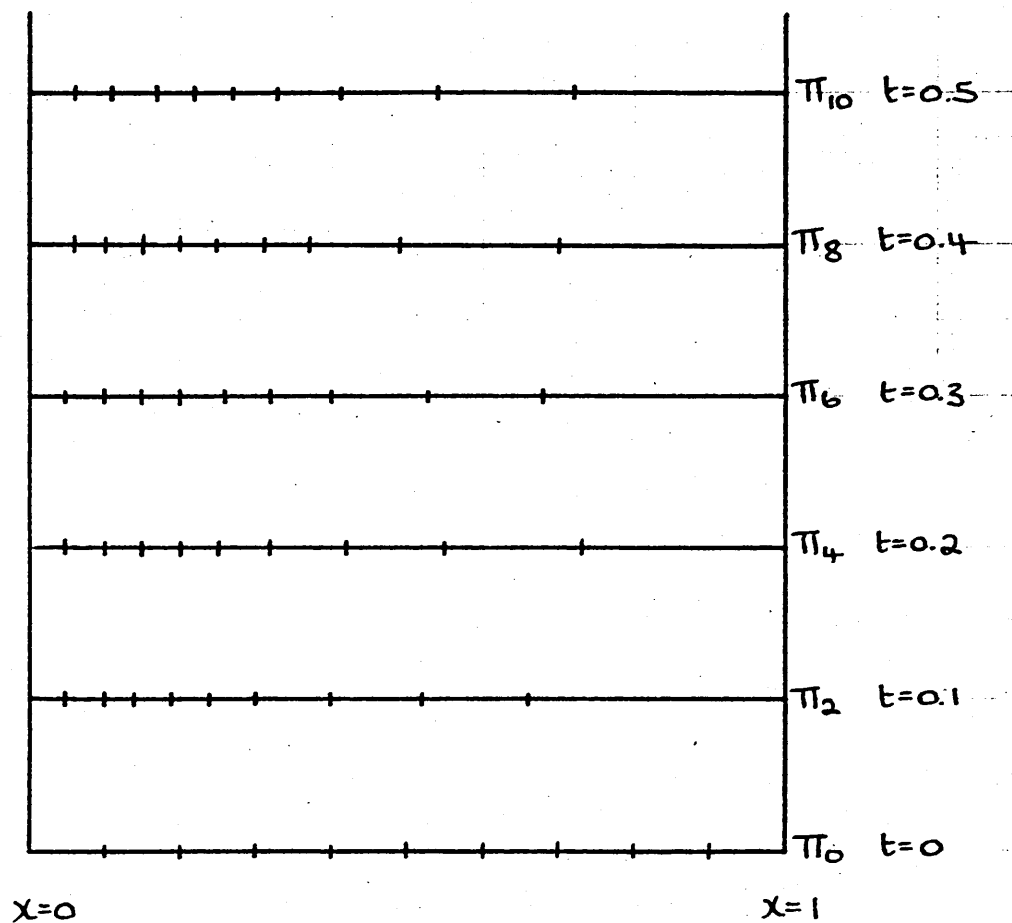Π_{2} t=0.1

Π_{0} t=0

X=0   X=1

Figure 21

Knot Partitions for Case Study 2.5 with a=10, k=0.05, $\theta = \frac{1}{2}$.
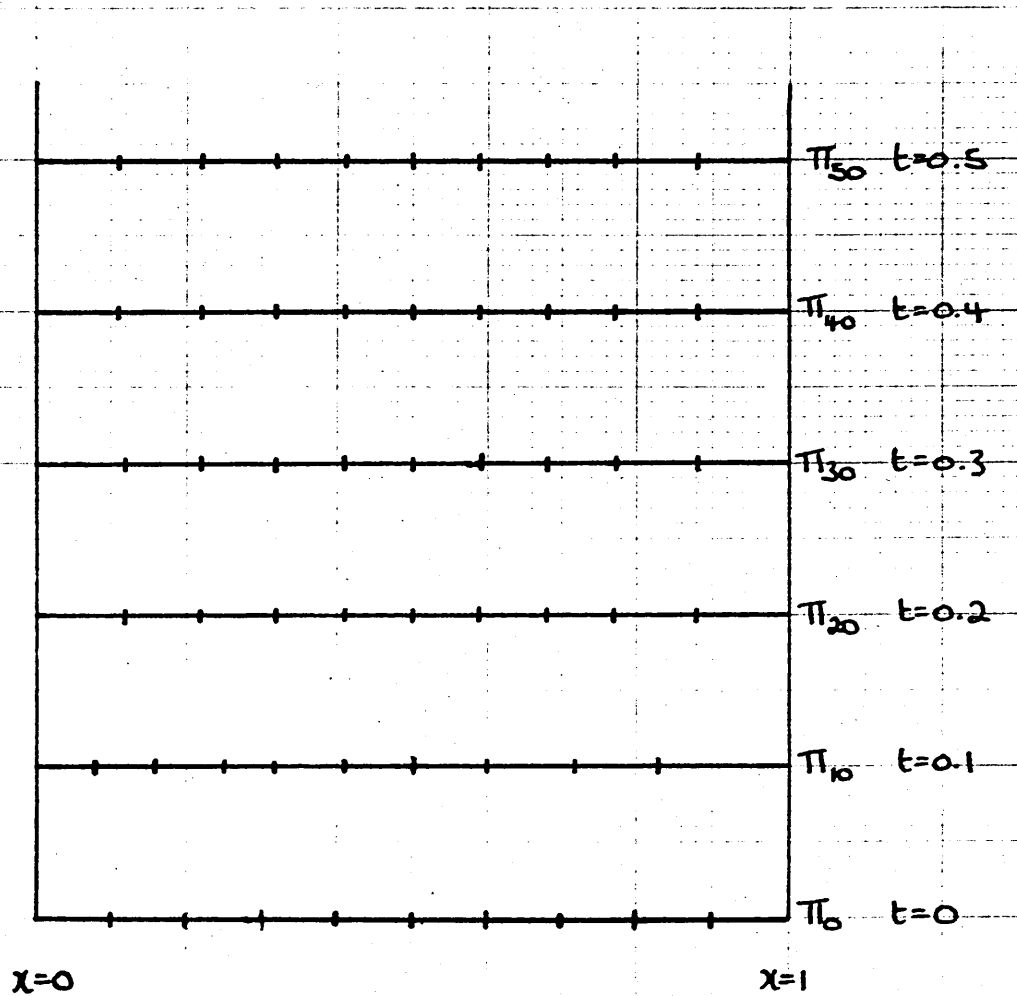
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Figure 22

Knot Partitions for Case STudy 2.5 with a=10, k=0.01, $\theta = \frac{1}{2}$.
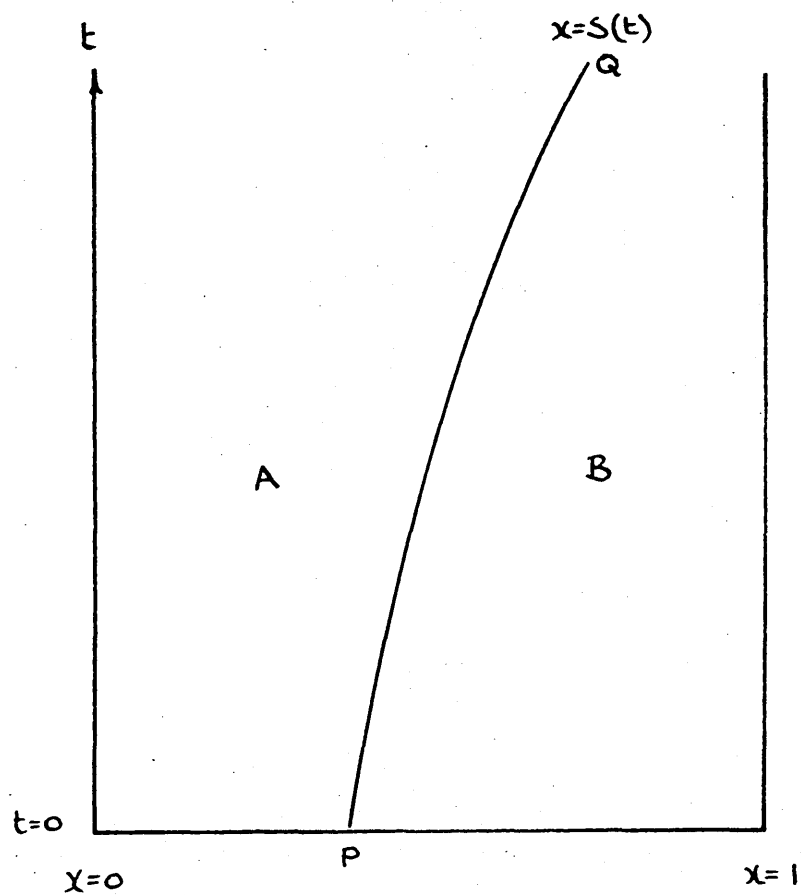
Figure 23

A Moving Boundary Problem

APPENDIX 1

Analytic Solution to Case Study 1.1

Here the analytic solution to the wave equation (6.2.1) is

derived by separating the variables. Letting u=XT in (6.2.1) and

dividing by XT we have

$$\frac{T''}{T} \quad = \quad \frac{X''}{X} \quad = \quad -k^2 \; . \qquad\qquad (AP1.1)$$

Rearranging (AP1.1) gives

$$T'' \; + \; k^2 T = 0 \qquad \text{and} \quad X'' \; + \; k^2 X \; = \; 0 \qquad\qquad (AP1.2)$$

which have the solutions

$$T = ASinkt + BCoskt \quad \text{and} \quad X = CSinkx + DCoskx \qquad\qquad (AP1.3)$$

respectively. The general solution to (6.2.1) thus has the form

$$u(x,t) = (ASinkt + BCoskt)(CSinkx + DCoskx) \qquad\qquad (AP1.4)$$

The constants, A, B, C, D and k are now evaluated using the imposed

boundary and initial conditions (6.2.2) − (6.2.4). From the left-

hand boundary condition of (6.2.2) we have

$$0 \; = \; (ASinkt + BCoskt)D \qquad\qquad (Ap.1.5)$$

implying D=0. Similarly the right-hand boundary condition of (6.2.2)

gives

$$\text{CSink} \quad = \quad - \text{DCosk} \qquad\qquad\qquad (\text{AP.1.6})$$

and thus $k = \pi$. Substituting the initial condition (6.2.3) into (AP1.4) yields

$$\text{Sin}\pi x \quad = \quad B(\text{CSinkx} + \text{DCoskx}). \qquad\qquad (\text{AP1.7})$$

Since D=0 and k=π then (AP1.7) suggest that BC=1. Finally, from the derivative initial condition (6.2.4) the following is derived

$$0 = \text{Ak}(\text{CSinkx} + \text{DCoskx}) \qquad\qquad\qquad (\text{AP1.8})$$

giving A=0. The general solution (AP1.4) thus becomes

$$u(x,t) = \text{Sin}\pi x \text{Cos}\pi t. \qquad\qquad\qquad (\text{AP1.9})$$

Analytic Solution to Case Study 1.2

The fourier series analytic solution to the wave equation (6.2.1)

is given by

$$u(x,t) = \sum_{n=1}^{\infty} a_n \, Sinn\pi x \, Cosn\pi t \qquad (AP2.1)$$

where

$$a_n = 2 \int_0^1 u(x,o) Sinn\pi x \, dx. \qquad (AP2.2)$$

In case study 1.2 the expression (AP2.2) becomes

$$a_n = 2 \int_0^1 (x^4 - x^5) \, Sinn\pi x \, dx \qquad (AP2.3)$$

which after successive integration by parts gives the relationship

$$a_n = 2 \left[\frac{24}{(n\pi)^5} - \left(\frac{-8}{(n\pi)^3} + \frac{96}{(n\pi)^5} \right) cosn\pi \right]. \qquad (AP2.4)$$

The analytic solution to (6.2.1) subject to (6.2.2), (6.3.1) and (6.3.2)

thus has the form

$$u(x,t) = \sum_{n=1}^{\infty} 2 \left[\frac{24}{(n\pi)^5} - \left(\frac{-8}{(n\pi)^3} + \frac{96}{(n\pi)^5} \right) cosn\pi \right] sinn\pi x \, Cosn\pi t.$$
$$\qquad (AP2.5)$$

APPENDIX 3.

Analytic Solution to Case Study 1.3

The analytic solution to (6.4.1) is easily derived by the method of separation of variables employed in Appendix 1. However, for illustrative purposes, the method of Laplace Transforms is used here.

Taking Laplace Transforms of (6.4.1) we have

$$s^2 U(x,s) - su(x,0) - \frac{\partial u}{\partial t}(x,0) = \frac{d^2 U}{dx^2} + cU \qquad \text{(AP3.1)}$$

which after substitution of the initial conditions (6.2.3) and (6.2.4) becomes

$$\frac{d^2 U}{dx^2} - (s^2 - c)U = - s\mathrm{Sin}\pi x. \qquad \text{(AP3.2)}$$

It is easily shown that the general solution of this differential equation has the form

$$U(x,s) = Ae^{\sqrt{s^2 - c}\,x} + Be^{-\sqrt{s^2 - c}\,x} + \frac{s\mathrm{Sin}\pi x}{\pi^2 + s^2 - c}. \qquad \text{(AP3.3)}$$

By taking Laplace Transforms of the boundary conditions (6.2.2) we find that the constants A and B are both zero and thus (AP3.2) has the solution

$$U(x,s) = \frac{s\mathrm{Sin}\pi x}{\pi^2 + s^2 - c}. \qquad \text{(AP3.4)}$$

Using inverse Laplace Transforms we therefore find

that the analytic solution to (6.4.1) subject to (6.2.2),

(6.2.3) and (6.2.4) is given by

$$u(x,t) = \sin\pi x \, \cos(\pi^2 - c)^{\frac{1}{2}} t. \qquad (AP3.5)$$

APPENDIX 4

Analytic Solution to Case Study 1.4

Using the method of separation of variables, (6.5.1) becomes
by letting $u = XT$

$$\frac{T'}{T} = \frac{X''}{X} = -k^2 \qquad (AP4.1)$$

and thus

$$T = Ae^{-k^2 t} \qquad (AP4.2)$$

and $\qquad X = BSinkx + Ccoskx \; . \qquad (AP4.3)$

The general solution to (6.5.1) therefore has the form

$$u(x,t) = Ae^{-k^2 t}(BSinkx + Ccoskx). \qquad (AP4.4)$$

From the boundary conditions (6.5.3) the general solution
(AP4.4) becomes

$$O = ACe^{-k^2 t} \qquad (AP4.5)$$

on x=0 and

$$O = Ae^{-k^2 t}(BSink + Ccosk) \qquad (AP4.6)$$

on x=1. Since $A \neq 0$, (AP4.5) gives C=0 and thus (AP4.6) becomes

$$BSink = 0 \; . \qquad (AP4.7)$$

If C=0 then $B \neq 0$ or u(x,t)=0 and hence (AP4.7) gives $k = \pi$.

Similarly, from the initial condition (6.5.2) the equation (AP4.4)
yields

$$\sin \pi x = A(B\sin kx + C\cos kx) \qquad \text{(AP4.8)}$$

and AB=1.

The general solution to the parabolic partial differential

(6.5.1) therefore has the form

$$u(x,t) = e^{-\pi^2 t} \sin \pi x. \qquad \text{(AP4.9)}$$

APPENDIX 5

Analytic Solution to Case Study 1.5

The steady-state solution to the equation (6.6.1) is when

$\frac{\partial u}{\partial t} = 0$, that is when $\frac{\partial^2 u}{\partial x^2} = 0$, and thus $u = A + Bx$. From the

boundary conditions (6.6.2) and (6.6.3) the constants A and B

are found to be A=1 and B=e^{-a} -1. Denoting the steady-state

solution by $u_o(x)$ we thus have

$$u_o(x) = 1 + (e^{-a}-1)x \quad . \tag{AP5.1}$$

The solutions to case study 1.5 are now defined by

$$u(x,t) = u_o(x) + v(x,t) \tag{AP5.2}$$

where $v(x,t)$ are solutions to the problem

$$\frac{\partial v}{\partial t} = \frac{\partial^2 v}{\partial x^2} \tag{AP5.3}$$

subject to

$$v(0,t) = v(1,t) = 0 \tag{AP5.4}$$

and $\quad v(x,0) = u(x,0) - u_o(x) = e^{-ax} - 1 + (1-e^{-a})x. \tag{AP5.5}$

The above problem is now in the more usual form for which the

fourier series solution is

$$v(x,t) = \sum_{n=1}^{\infty} b_n Sinn\pi x \ e^{-n^2 \pi^2 t} \tag{AP5.6}$$

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where

$$b_n = 2 \int_0^1 v(x,0) \sin n\pi x \, dx. \qquad \text{(AP5.7)}$$

using (AP5.5) the integral (AP5.7) becomes

$$b_n = 2 \int_0^1 (e^{-ax} - 1 + (1-e^{-a})x) \sin n\pi x \, dx. \qquad \text{(AP5.8)}$$

which can be shown to have the solution

$$b_n = \frac{2}{n\pi} (e^{-a} \cos n\pi - 1) \left(\frac{a^2}{(n\pi)^2 + a^2} \right). \qquad \text{(AP5.9)}$$

The analytic solution to (6.5.1) subject to (6.6.1), (6.6.2) and

(6.6.3) is therefore given by the expression

$$u(x,t) = 1 + (e^{-a} - 1)x$$

$$+ \sum_{n=0}^{\infty} \frac{2}{n\pi} \left(e^{-a} \cos n\pi - 1 \right) \left(\frac{a^2}{(n\pi)^2 + a^2} \right) \sin n\pi x \, e^{-n^2 \pi^2 t} \qquad \text{(AP5.10)}$$

The numerical evaluation of (AP5.10) is complicated by the presence

of the $\sin n\pi x$ term. In evaluating the summation it is usual to sum

terms until a particular term is less than a specified magnitude.

This is difficult in this case, since $\sin n\pi x = 0$ for certain values

of n and x, and thus significant terms for larger n will be ignored.

In our computations this problem has been overcome by examining terms

after those in which $\sin n\pi x = 0$.

An additional danger is also encountered when n is large since in such

cases $e^{-n^2 \pi^2 t}$ becomes too small for computer arithmetic operations.

REFERENCES

J H AHLBERG, E N NILSON and J L WALSH, The Theory of Splines
and their Application, Academic Press, London (1967)

E L ALBASINY and W D HOSKINS, Cubic Spline Solutions to Two-
Point Boundary Value Problems, Comput.J.12(1969)151-153

W F AMES, Numerical Methods for Partial Differential Equations,
Nelson and Sons (1977)

G H BEHFOROOZ and N PAPAMICHAEL, End Conditions for Cubic Spline
Interpolation, J.Inst.Maths.Applics. 23(1979)355-366

W G BICKLEY, Piecewise Cubic Interpolation and Two-Point Boundary
Value Problems, Comput.J.11(1968)206-208

G BIRKHOFF and C DE BOOR, Piecewise Polynomial Interpolation and
Approximation, In Approximation of Functions edited by
H L Garabedian, Elsevier, Amsterdam (1965)164-190

F G BLOTTNER, Non-Uniform Grid Methods for Turbulent Boundary
Layers, Proc.Fourth Int.Conf.on Numerical Methods in
Fluid Dynamics, Lecture Notes in Physics 35, Springer-Verlag
(1975)

H G BURCHARD, Splines (with optimal knots) are better, J.Applicable
Analysis 3(1974)309-319

I CHRISTIE, D F GRIFFITHS, A R MITCHELL and O C ZIENKIEWICZ,
Finite Element Methods for Second Order Differential
Equations with Significant First Derivatives, Int.J.
Numer.Meth.Eng. 10(1976)1389-1396

R COURANT, K FRIEDRICHS and H LEWY, Über die partiellen
Differenzengleichungen der Mathematischen Physik, Math.
Ann.100(1928)32-74, English translation by Phyllis Fox,
On the partial difference equations of Mathematical
Physics, IBM Journal 11(1967)215-234

M G COX, An Algorithm for Spline Interpolation, J.Inst.Maths.
Applics. 15(1975)95-108

S H CRANDELL, An Optimum Implicit Recurrence Formula for the
Heat Conduction Equation, Qtly.Apl.Maths. 13(1955)318-320

J CRANK and R S GUPTA, A Moving Boundary Problem Arising from the
Diffusion of Oxygen in Absorbing Tissue, J.Inst.Maths.Applics.
10(1972a)19-33

J CRANK and R S GUPTA, A Method for Solving Moving Boundary
    Problems in Heat Flow Using Cubic Splines or Polynomials,
    J.Inst.Maths.Applics. 10(1972b)296-304

J CRANK and P NICOLSON, A Practical Method for the Numerical
    Evaluation of Solutions of Partial Differential Equations
    of the Heat Conduction Type, Proc.Camb.Phil.Soc.
    43(1947)50-67

A R CURTIS, The Approximation of a Function of One Variable by
    Cubic Splines, in Numerical Approximations to Functions
    and Data edited by J G Hayes, Athlone Press, London (1970)28-42

A R CURTIS and M J D POWELL, Using Cubic Splines to Approximate
    Functions of One Variable to Prescribed Accuracy,
    AERE Harwell Report No. AERE-R5602, HMSO(1967)

H J CROWDER and C DALTON, Errors in the Use of Nonuniform Mesh
    Systems, J.Comp.Physics 7(1971)32-45

C DE BOOR, Good Approximation by Splines with Variable Knots, In
    Spline Functions and Approximation Theory edited by A Meir
    and A Sharma, Birkhaüser Verlag, Basel (1973)57-72

C DE BOOR, Good Approximation by Splines with Variable Knots II,
    In Numerical Solution of Differential Equations edited by
    G A Watson, Lecture Notes in Math.No.363, Springer-Verlag
    (1974) 12-20

C DE BOOR, A Practical Guide to Splines, Springer-Verlag,
    New York (1978)

C DE BOOR and J R RICE, Least-Squares Cubic Spline Approximation
    II - Variable Knots, Computer Science Department Technical
    Report 21, Purdue University (1968)

C DE BOOR and B SWARTZ, Collocation at Gaussian Points, SIAM J.
    Numer.Anal.10(1973)582-606

D S DOBSON, Optimal Order Approximation by Polynomial Spline
    Functions, PhD Thesis, Purdue Univ. Lafayette, Ind. (1972)

J DOUGLAS, The Solution of the Diffusion Equation by a High Order
    Correct Difference Equation, J.Math.Phys. 35(1956)145-151

J DOUGLAS and T M GALLIE, Variable Time Steps in the
   Solution of the Heat Flow Equation by a Difference
   Equation, Proc.Amer.Soc. 6(1955)787-793

M E A EL-TOM, Spline Function Approximations to the Solution
   of Singular Volterra Integral Equations of the Second
   Kind, J.Inst.Maths.Applics. 14(1974)303-309

M E A EL-TOM, Application of Spline Functions to Systems of
   Volterra Integral Equations of the First and Second
   Kinds, J.Inst.Maths.Applics. 17(1976)295-310

R E ESCH and W L EASTMAN, Computational Methods for Best
   Spline Function Approximation, J.Approx.Theory 2(1969)
   85-96

L FOX, Numerical Solution of Ordinary and Partial Differential
   Equations, Pergamon Press, London (1962)

D J FYFE, The Use of Cubic Splines in the Solution of Two-Point
   Boundary Value Problems, Comput.J.12(1969)188-192

T N E GREVILLE, Introduction to Spline Functions, In Theory and
   Applications of Spline Functions edited by T N E Greville,
   Academic Press, New York (1969)1-35

D F GRIFFITHS, The Stability of Finite Difference Approximations
   to Nonlinear Partial Differential Equations, Bull.IMA
   18(1982)210-215

J G HAYES and J HALLIDAY, The Least-Squares Fitting of Cubic
   Spline Surfaces to General Data Sets, J.Inst.Maths.Applics.
   14(1974)89-103

M K JAIN and T AZIZ, Spline Function Approximation for
   Differential Equations, Comp.Meth.Appl.Mech.and Eng. 26(1981)
   129-143

P C JAIN and D N HOLLA, General Finite Difference Approximation
   for the Wave Equation with Variable Coefficients using a
   Cubic Spline Technique, Comp.Meth.Appl.Mech.and Eng. 15
   (1978)175-180

I P JONES and C P THOMPSON, On the Use of Nonuniform Grids in
   Finite Difference Calculations, AERE Harwell Report
   No. AERE-R9765, HMSO(1980)

E KALNAY DE RIVAS, On the Use of Nonuniform Grids in
   Finite Difference Equations, J.Comp.Physics 10(1972)
   202-210

D KERSHAW, Two Interpolatory Cubic Splines, J.Inst.Maths.
   Applics. 11(1973)329-333

A K A KHALIFA and J C EILBECK, Collocation with Quadratic
   and Cubic Splines, IMA J.Numer.Anal. 2(1982)111-121

F R LOSCALZO, An Introduction to the Application of Spline
   Functions to Initial Value Problems, in Theory and
   Application of Spline Functions edited by T N E Greville
   Academic Press, New York (1969)

F R LOSCALZO and T D TALBOT, Spline Function Approximation
   for Solution of Ordinary Differential Equations,
   SIAM J.Numer.Anal. 4(1967)433-445

M LOTKIN, The Calculation of Heat Flow in Melting Solids,
   Q.Appl.Math.18(1960)79-85

D E McCLURE, Feature Selection for the Analysis of Line
   Patterns, Ph.D.,Thesis, Brown Univ., Providence,
   R.I. (1970)

S McKEE, High Accuracy A.D.I. Methods for Hyperbolic Equations
   with Variable Coefficients, J.Inst.Maths.Applics. 11
   (1973)105-109

G H MEYER, The Numerical Solution of Stefan Problems with Front-
   Tracking and Smoothing Methods, Brunel University Report
   TR/62(1976)

G MICULA, Approximate Solution of the Differential Equation
   y" = f(x,y) with Spline Functions, Maths of Comp. 27(1973)
   807-816

A R MITCHELL, Computational Methods in Partial Differential
   Equations, Wiley, Aberdeen (1969)

A R MITCHELL and D F GRIFFITHS, The Finite Difference Method
   in Partial Differential Equations, Wiley, Chichester,
   New York (1980)

W D MURRAY and F LANDIS, Numerical and Machine Solutions of
   Transient Heat-Conduction Problems involving Melting
   or Freezing, J.Heat Transfer 81(1959)106-112

G G O'BRIEN, M A HYMAN and S KAPLAN, A Study of the Numerical
    Solution of Partial Differential Equations, J.Math.Phys.
    29(1951)223-251

J R OCKENDON and W R HODGKINS (Eds), Moving Boundary Problems
    in Heat Flow and Diffusion, Clarendon Press, Oxford (1975)

M M PALA and P SPANO, A Cubic Spline Technique for a
    Parabolic Equation of Higher than the Second Order,
    Bollettino U.M.I. 15(1978)560-570

N PAPAMICHAEL and J R WHITEMAN, A Cubic Spline Technique
    for the One-Dimensional Heat Conduction Equation,
    J.Inst.Maths.Applics. 11(1973)111-113

N PAPAMICHAEL and A J WORSEY, End Conditions for Improved
    Cubic Spline Derivative Approximations, J.Comp.
    Appl.Maths. 7(1981)101-109

F PATRICIO, Cubic Spline Functions and Initial Value Problems,
    BIT 18(1978)342-347

C E PEARSON, On a Differential Equation of Boundary Layer
    Type, J.Math.and Phys. 47(1968)134-154

G M PHILLIPS, Error Estimates for Best Polynomial Approximation,
    In Approximation Theory edited by A Talbot, Academic Press,
    London (1970)1-6

H S PRICE, J C CAVENDISH and R S VARGA, Numerical Methods of
    Higher-Order Accuracy for Diffusion-Convection Equations,
    Soc.Pet.Eng.J. 8(1968)293-303

G F RAGGETT, On the Solution of Hyperbolic Partial Differential
    Equations Using Cubic Splines, Paper presented at the
    International Congress of Mathematicians, Vancouver,
    Canada (1974)

G F RAGGETT, J A R STONE and S J WISHER, The Cubic Spline Solution
    of Hyperbolic Partial Differential Equations with Variable
    Coefficients and Generalised Boundary Conditions, Research
    Report MS/01, Sheffield City Polytechnic (1975)

G F RAGGETT, J A R STONE and S J WISHER, The Cubic Spline
    Solution of Practical Problems Modelled by Hyperbolic
    Partial Differential Equations, Comp.Meth.Appl.Mech.and
    Eng. 8(1976)139-151

G F RAGGETT and P D WILSON, A Fully Implicit Finite Difference
    Approximation to the One-Dimensional Wave Equation Using
    a Cubic Spline Technique, J.Inst.Maths.Applics.14(1974)
    75-77

G F RAGGETT and S J WISHER, Variable Knot Placement in the
    Cubic Spline Solution of Hyperbolic Partial Differential
    Equations - A Local Method, Research Report MS/04,
    Sheffield City Polytechnic (1979a)

G F RAGGETT and S J WISHER, Variable Knot Placement in the
    Cubic Spline Solution of Hyperbolic Partial Differential
    Equations - A Global Method, Research Report MS/05,
    Sheffield City Polytechnic (1979b)

J R RICE, On the Degree of Convergence on Non-Linear Spline
    Approximation, In Approximations with Special Emphasis
    on Spline Functions edited by I J Schoenberg, Academic
    Press, New York (1969) 349-365

L F RICHARDSON, The Approximate Arithmetical Solution by
    Finite Differences of Physical Problems Involving
    Differential Equations, Phil.Trans.Roy.Soc.London,
    Series A, 210(1910) 307-357

R D RICHTMYER and K W MORTON, Difference Methods for
    Initial-Value Problems, Interscience, New York (1967)

S G RUBIN and R A GRAVES, Viscous Flow Solutions with a
    Cubic Spline Approximation, Computers and Fluids
    3(1975) 1-36

S G RUBIN and P KHOSLA, Higher-Order Numerical Solutions
    Using Cubic Splines, AIAA Journal 14(1976) 851-858

V K SAUL'YEV, Integration of Equations of Parabolic Type
    by the Method of Nets, Pergamon Press, London (1964)

S S SASTRY, Finite Difference Approximations to One-Dimensional
    Parabolic Equations using a Cubic Spline Technique, J.Comp.
    Appl.Maths 2(1976) 23-26

I J SCHOENBERG, Contributions to the Problem of Approximation
    of Equidistant Data by Analytic Functions, Quart.
    Appl.Math.4(1946), Part A 45-99, Part B 112-141

M H SCHULTZ, Spline Analysis, Prentice-Hall (1973)

L L SCHUMAKER, Some Algorithms for the Computation of
    Interpolating and Approximating Spline Functions,
    In Theory and Applications of Spline Functions edited
    by T N E Greville, Academic Press, New York (1969)
    87-102

J L SIEMIENIUCH and I GLADWELL, Analysis of Explicit Difference
    Methods for a Diffusion-Convection Equation, Int.J.Numer.
    Meth.Eng. 12(1978)899-916

D E SPALDING, A Novel Finite Difference Formulation for
    Differential Expressions involving both First and Second
    Derivatives, Int.J.Numer.Meth.Eng. 4(1972)551-559

O B WIDLUND, Stability of Parabolic Difference Schemes in
    the Maximum Norm, Numer.Math. 8(1966)186-202

S J WISHER, On the Use of Splines in the Numerical Solution
    of Hyperbolic Partial Differential Equations, M.Phil.
    Thesis, Sheffield City Polytechnic (1977)

G WOODFORD, Finite Difference Methods with Application to the
    Cavity Problem, PhD Thesis, Australian National University
    (1975)