Higher-Order Finite-Difference Methods for Partial Differential Equations

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To my parents and my children

Shozab Ali, Tansheet Ali and Aisha Tasneem.

Abstract

This thesis develops two families of numerical methods, based upon rational approximations having distinct real poles, for solving first- and second-order parabolic/ hyperbolic partial differential equations. These methods are third- and fourth-order accurate in space and time, and do not require the use of complex arithmetic. In these methods first- and second-order spatial derivatives are approximated by finite-difference approximations which produce systems of ordinary differential equations expressible in vector-matrix forms. Solutions of these systems satisfy recurrence relations which lead to the development of parallel algorithms suitable for computer architectures consisting of three or four processors. Finally, the methods are tested on advection, advection-diffusion and wave equations with constant coefficients.

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Chapter 1

Preliminaries

1.1 Introduction

With the increasing availability of powerful computing machines and the improvement in numerical techniques finite difference methods are being used more and more in the solution of physical problems that arise in various branches of continuum physics such as heat flow, diffusion, fluid dynamics, magneto-fluid dynamics, electromagnetism, wave mechanics, radiation transfer, neutron transfer, elastic vibrations ([1], [33]), medical fluid dynamics, bioengeering, soil physics and chemistry [1] and population dynamics [16]. In the description of these physical problems partial differential equations and systems of such equations appear which involve two or more independent variables that determine the behaviour of the dependent variable.

It is often useful to classify partial differential equations into two kinds: *steady-state* equations (for example, the Poisson equation and the biharmonic equation) and *evolutionary equations* which model systems that undergo change as a function of time and they are important *inter alia* in the description of wave phenomena, thermodynamics, diffusive processes and population dynamics [16].

According to a natural classification of partial differential equations depending upon ***characteristic directions*** a partial differential equation may be *elliptic, parabolic or hyperbolic* (see [35], [41], *etc*). Elliptic equations are of the steady-state type whilst both parabolic and hyperbolic partial differential equations are evolutionary (unsteady).

The method of characteristics (see [35], [41], *etc*) is undoubtedly the most effective method for solving hyperbolic equations in one space dimension, but loses its impact in higher dimensions where it is less satisfactory [5], and where, therefore, finite differences still have a role to play. So in the last two decades much attention has been given in the literature to the development, analysis and implementation of stable and accurate methods for the numerical solution of partial differential equations with mixed initial and boundary conditions specified.

There are many forms of model hyperbolic partial differential equations that are used in analysing various finite difference methods. These range from simple one-dependent variable first-order partial differential equations through multiple dependent-variable second-order partial differential equations with as many as three space variables [23]; for example, finite-difference methods for the wave equation are used in [4], [9], [11], [12], [24], [27], [30], [34], [40], [47], [49], and [50] and accurate methods for first-order hyperbolic partial differential equations are developed in [5], [20] and [31].

In this thesis third- and fourth-order numerical methods for the solution of hyperbolic partial differential equations which do not require complex arithmetic will be developed and tested on well-known problems with exact solutions known.

1.2 Method of Lines

Covering the region, in which a numerical solution is to be solved, by a rectangular grid with sides parallel to the axes and then replacing the spatial derivatives in the partial differential equation by their finite-difference approximations, thus transforming the partial differential equations, is called the *Method of Lines.* Time-dependent problems in Partial Differential Equations (PDEs) are often solved by the Method of Lines (MOL). By this method the initial/boundary-value problem is transformed into an initial-value in system form; it can be written in vector-matrix form and its solution satisfies a recurrence relation. Then numerical methods are developed using suitable approximations in this recurrence relation.

1.3 Rational Approximations to $\exp(t)$

Several algorithms for the numerical solution of partial differential equations can be generated through an approximation to the elementary function appearing in the recurrence relation, which is satisfied by the exact solution of the initial value problem. The use of rational functions for this purpose has a long and rich history (see, for example, [4], [5], [27], [32], [38], [39], [47], [54] and referrences therein). Perhaps the most well known and frequently used are the Padé approximants due to their order and/or stability properties. But methods for solving partial differential equations corresponding to higher-order Padé approximations entail the use of complex arithmetic in a splitting context. Third- and fourth-order,L-acceptable rational approximations to $\exp(t)$, introduced by Taj and Twizell in [38] and [39], which possess real and distinct poles are given, for a real scalar t, as

$$E_3(t) = \frac{1 + (1-a)t + (\frac{1}{2} - a + b)t^2}{1 - at + bt^2 - (\frac{1}{6} - \frac{a}{2} + b)t^3} \qquad (1.\ 1)$$

and

$$E_4(t) = \frac{1 + (1-a)t + (\frac{1}{2} - a + b)t^2 + (\frac{1}{6} - \frac{a}{2} + b - c)t^3}{1 - at + bt^2 - ct^3 + (-\frac{1}{24} + \frac{a}{6} - \frac{b}{2} + c)t^4} \qquad (1.\ 2)$$

in which a, b and c are real numbers, respectively. The error constants for these rational approximations are

$$-\frac{1}{8} + \frac{a}{3} - \frac{b}{2}$$

and

$$-\frac{1}{30} + \frac{a}{8} - \frac{b}{3} + \frac{c}{2}$$

respectively. These approximations to $\exp(t)$ will play a particular rôle in later chapters.

1.4 Notations

Usually the theoretical solution of a hyperbolic partial differential equation is denoted by u and the theoretical solution of a finite-difference equation is denoted by U, while the computed solution is denoted by $\tilde{U}$. The position at which the solution is taken is shown by appropriate indices, for example, u_m^n denotes the theoretical solution of a certain hyperbolic partial differential equation in one space dimension at mesh point $(x,t) = (mh, nl)$ and U_m^n denotes the theoretical solution of a finite-difference scheme at the same mesh point. A description of each mesh used in this thesis is given as it is introduced.

1.5 Analysis of Difference Schemes

1.5.1 Local Truncation Error

Suppose that a hyperbolic equation is written in the form

$$L(u) = 0$$

with exact solution u, and let $F(U) = 0$ represent the approximating finite-difference equation with exact solution U. Replacing U by u at each mesh point occurring in the finite-difference scheme, and carrying out Taylor expansions about (mh, nl), the value of $l^{-1}F_{m,n}(u) - L(u_m^n)$ (in case of first-order hyperbolic equation) or $l^{-2}F_{m,n}(u) - L(u_m^n)$ (in case of second-order hyperbolic equation) is the **local truncation error** at the mesh point (mh, nl); that is, the local truncation error is the difference between the finite-difference scheme and the differential equation it replaces. The order of the scheme is the order of the lowest-order terms in h and l.

1.5.2 Local Discretization Error

The local discretization error is the difference between the theoretical solution of the differential and difference equations and is represented at the mesh point (mh, nl) by

$$z_m^n = u_m^n - U_m^n.$$

1.5.3 Consistency

A difference approximation to a hyperbolic equation is **consistent** if

$$\textit{local truncation error} \longrightarrow 0$$

as space and time steps are refined.

1.5.4 Stability

A finite difference scheme used to solve a *PDE* is said to be stable if the difference between the theoretical solution of the difference equation and the solution actually obtained at the mesh point (mh, nl) remains bounded as n increases, for fixed h, l and h, $l \to 0$ for a fixed value of $t = nl$. The concept of stability is concerned with the boundedness of the solution of the finite-difference equation (Twizell [41]) and this is examined by finding conditions under which

$$Z_m^n = U_m^n - \tilde{U}_m^n$$

remains bounded as n increases for fixed h, l.

There are two methods which are commonly used for examining this notion of stability of a finite difference scheme for hyperbolic partial differential equations namely, the von Neumann Method and the Matrix Method.

(a) The von Neumann Method

Consider the local discretization error

$$Z_m^n = U_m^n - \tilde{U}_m^n$$

and introduce the error function at a given time level t

$$G(x, t) = e^{\alpha t} e^{i\beta x}$$

where β is real and α is, in general, complex, such that

$$Z_m^n = G(x, t) \neq 0.$$

To investigate the error propagation as t increases, it is necessary to find a solution of the finite-difference equation which reduces to $e^{i\beta x}$ when $t = 0$.

Let such a solution be

$$e^{\alpha t}e^{i\beta x} = e^{\alpha nl}e^{i\beta mh}.$$

The original error component will not grow with time if

$$| e^{\alpha l} | \leq 1$$

for all α. This is von Neumann's necessary condition for stability. Here the quantity

$$\xi = e^{\alpha l}$$

is called the *amplification factor.*

(b) The Matrix Method

The totality of difference equations connecting values of $\mathbf{U}$ at two neighbouring time levels can be written in the matrix form

$$D\mathbf{U}^{n+1} = B\mathbf{U}^n + C\mathbf{U}^{n-1} + \mathbf{b}^n \qquad (1.3)$$

where $\mathbf{U}^k (k = n-1, n, n+1)$ denotes the column vector

$$[U_1^k, U_2^k, \ldots, U_N^k]^T,$$

$\mathbf{b}^n$ is a vector which depends on the boundary conditions and D, B, C are square matrices of order N (where N is the number of mesh points at each time level). In the case of a differential equation with constant coefficients the matrices D, B, C are constant, in the case of a variable coefficients problems, the matrices D, B, C are evaluated at times $(n+1)l$, nl, $(n-1)l$ respectively. Writing (1.1) in the form

$$\mathbf{U}^{n+1} = D^{-1}B\mathbf{U}^n + D^{-1}C\mathbf{U}^{n-1} + D^{-1}\mathbf{b}^n$$

follows that a perturbation $\mathbf{Z}^0$ of the initial conditions will satisfy

$$\mathbf{Z}^{n+1} = D^{-1}B\mathbf{Z}^n + D^{-1}C\mathbf{Z}^{n-1}.$$

This may be written as

$$\begin{bmatrix} \mathbf{Z}^{n+1} \\ \mathbf{Z}^{n} \end{bmatrix} = \begin{bmatrix} D^{-1}A & D^{-1}C \\ I & O \end{bmatrix} \begin{bmatrix} \mathbf{Z}^{n} \\ \mathbf{Z}^{n-1} \end{bmatrix} \qquad (1.4)$$

which is of the form

$$\mathbf{E}^{n+1} = W\mathbf{E}^{n}$$

where $\mathbf{E}^{n+1} = [(\mathbf{Z}^{n+1})^T, (\mathbf{Z}^n)^T]^T$. It follows that

$$\| \mathbf{E}^{n+1} \| \leq \| W \| \| \mathbf{E}^{n} \|,$$

where $\| \,.\, \|$ denotes a suitable norm. The necessary and sufficient condition for the stability of a scheme based on a constant time step and proceeding indefinitely in time is

$$\| W \| \leq 1,$$

for all n, and so the stability condition for the difference scheme, used in this way, depends on obtaining a suitable estimate for $\| W \|$. When W is symmetric,

$$\| W \|_2 = \max_s | \lambda_s |$$

where $\lambda_s (s = 1, 2, \ldots, N)$ are the eigenvalues of W and $\| \,.\, \|_2$ denotes the L_2-norm. Here, $\max_s | \lambda_s |$ is the spectral radius of W and W is called the *amplification matrix.*

1.5.5 Convergence

A finite-difference method for hyperbolic partial differential equations is said to be convergent if the local discretization error

$$z_m^n = u_m^n - U_m^n,$$

at the *fixed* mesh point (x_m, t_n), tends to zero as the mesh is refined by letting $h, l \rightarrow 0$ simultaneously. In carrying out the convergence analysis, it may be convenient to assume that h and l do not tend to zero independently but according to a relationship of the form

$$l = rh^{\alpha},$$

where r is a constant and $\alpha \geq 1$ is some parameter.

Chapter 2

Third-Order Numerical Methods for the Advection Equation

2.1 Introduction

There are many finite-difference approximations which can be used to develop numerical methods for first-order hyperbolic partial differential equations of the type

$$\frac{\partial u(x,t)}{\partial t} + \lambda \frac{\partial u(x,t)}{\partial x} = 0, \quad \lambda > 0, \qquad (2.1)$$

with appropriate initial and boundary conditions specified. For example, central-difference approximations for u_t and u_x, or alternatively a forward-difference approximation for u_x and a central-difference approximation for u_t,*etc*, can be used. But in this chapter only the space derivative in the partial differential equation (2.1) is replaced by new third-order finite-difference approximations resulting in a system of first-order ordinary differential equations. The solution of this system satisfies a recurrence relation. The accuracy in time is controlled by choosing a third-order approximation (introduced by Taj and Twizell [38]) to the matrix exponential function and afterwards a parallel algorithm is developed and tested on well-known problems with exact solutions are already known in the literature.

2.2 The Model Problem

A typical problem in applied mathematics consisting of the first-order hyperbolic partial differential equation is the advection equation. This initial/ boundary-value problem (IBVP) is given by

$$\frac{\partial u(x,t)}{\partial t} + \lambda \frac{\partial u(x,t)}{\partial x} = 0, \quad \lambda > 0, x > 0, \quad t > 0 \qquad (2.2)$$

with the boundary conditions

$$u(0,t) = f(t), \quad t > 0 \qquad (2.3)$$

and the initial condition

$$u(x,0) = g(x), \quad x \geq 0 \qquad (2.4)$$

where $g(0) = f_0(0)$ and $g(x)$ is a given continuous function of x. There will exist a discontinuity between the initial-condition and the boundary-condition at origin if

$$g(0) \neq f_0(0).$$

2.3 The Method

Suppose that the solution $u(x,t)$ of $\{(2.2)\text{-}(2.4)\}$ is to be determined in some arbitrary region $R = [0 \leq x \leq X] \times [t > 0]$. Dividing the interval $[0, X]$ into N subintervals each of width h, so that $Nh = X$, and the time variable

t into time steps each of length l gives a rectangular mesh of points with co-ordinates

$$(x_m, t_n) = (mh, nl)$$

($m = 0, 1, 2, \ldots, N$ and $n = 0, 1, 2, \ldots$) covering the region $R = [0 < x < X] \times [t > 0]$ and its boundary ∂R consisting of the lines $x = 0$, $x = X$ and $t = 0$.

To approximate the space derivative in (2.2) to third-order accuracy at some general point (x, t) of the mesh, assume that it may be replaced by the four-point formula

$$\begin{aligned} \frac{\partial u(x,t)}{\partial x} &= \frac{1}{h}\{a\,u(x,t) + b\,u(x-h,t) + c\,u(x-2h,t) \\ &+ d\,u(x-3h,t)\}. \end{aligned} \tag{2.5}$$

Expanding the terms $u(x-h,t)$, $u(x-2h,t)$ and $u(x-3h,t)$ as Taylor series about (x,t) in (2.5) gives

$$\begin{aligned} h\frac{\partial u(x,t)}{\partial x} &= (a+b+c+d)\,u(x,t) \\ &+ (-b-2c-3d)\,h\frac{\partial u(x,t)}{\partial x} \\ &+ \frac{1}{2!}(b+4c+9d)\,h^2\frac{\partial^2 u(x,t)}{\partial x^2} \\ &+ \frac{1}{3!}(-b-8c-27d)\,h^3\frac{\partial^3 u(x,t)}{\partial x^3} \\ &+ \frac{1}{4!}(b+16c+81d)\,h^4\frac{\partial^4 u(x,t)}{\partial x^4} \\ &+ O(h^5) \ \ as \ \ h \to 0. \end{aligned} \tag{2.6}$$

Equating powers of $h^i (i = 0, 1, 2, 3)$ in (2.6) gives

$$\begin{aligned} a+b+c+d &= 0, \\ -b-2c-3d &= 1, \end{aligned}$$

$$b + 4c + 9d = 0, \qquad (2.7)$$
$$-b - 8c - 27d = 0.$$

The solution of the linear system (2.7) is

$$a = \frac{11}{6}, \quad b = -3, \quad c = \frac{3}{2}, \quad d = \frac{-1}{3}. \qquad (2.8)$$

Thus

$$\begin{aligned} \frac{\partial u(x,t)}{\partial x} &= \frac{1}{6h}\{-2u(x-3h,t) + 9u(x-2h,t) - 18u(x-h,t) \\ &+ 11u(x,t)\} + \frac{h^3}{4}\frac{\partial^4 u(x,t)}{\partial x^4} + O(h^4) \;\; as \;\; h \to 0 \qquad (2.9) \end{aligned}$$

is the desired third-order approximation to the first-order space derivative at (x,t).

Equation (2.9) is valid only for $(x,t) = (x_m, t_n)$ with $m = 3, 4, \ldots, N$. To attain the same accuracy at the end points (x_1, t_n) and (x_2, t_n), special formulae must be developed which approximate $\partial u(x,t)/\partial x$ not only to third-order but also with dominant error term $\frac{1}{4}h^3\partial^4 u(x,t)/\partial x^4$ for $x = x_1, x_2$ and $t = t_n$. To achieve both of these, five-point formulae will be needed in each case. Consider, then, the approximation to $\partial u(x,t)/\partial x$ at the point $(x,t) = (x_1, t_n)$: let

$$\begin{aligned} 6h\frac{\partial u(x,t)}{\partial x} &= a\,u(x-h,t) + b\,u(x,t) + c\,u(x+h,t) \\ &+ d\,u(x+2h,t) + e\,u(x+3h,t) + \frac{3}{2}h^4\frac{\partial^4 u(x,t)}{\partial x^4} \\ &+ O(h^5) \;\; as \;\; h \to 0. \qquad (2.10) \end{aligned}$$

Then expanding the terms $u(x-h,t)$, $u(x+h,t)$, $u(x+2h,t)$ and $u(x+3h,t)$ as Taylor series about the point (x,t) gives

$$6h\frac{\partial u(x,t)}{\partial x} = (a + b + c + d + e)\,u(x,t)$$

$$
\begin{aligned}
&+ \quad (-a+c+2d+3e)\,h\frac{\partial u(x,t)}{\partial x} \\
&+ \quad \frac{1}{2!}(a+c+4d+9e)\,h^2\frac{\partial^2 u(x,t)}{\partial x^2} \\
&+ \quad \frac{1}{3!}(-a+c+8d+27e)\,h^3\frac{\partial^3 u(x,t)}{\partial x^3} \\
&+ \quad \frac{1}{4!}(a+c+16d+81e+36)\,h^4\frac{\partial^4 u(x,t)}{\partial x^4} \\
&+ \quad O(h^5) \;\; as \;\; h \to 0. \qquad (2.11)
\end{aligned}
$$

Equating powers of $h^i (i = 0, 1, 2, 3, 4)$ in (2.11) gives

$$
\begin{aligned}
a+b+c+d+e &= 0, \\
-a+c+2d+3e &= 6, \\
a+c+4d+9e &= 0, \qquad (2.12) \\
-a+c+8d+27e &= 0, \\
a+c+16d+81e &= -36.
\end{aligned}
$$

The solution of the linear system (2.12) is

$$
a=-3, \quad b=1, \quad c=0, \quad d=3, \quad e=-1. \qquad (2.13)
$$

Thus, at the mesh point (x_1, t_n), the desired third-order approximation to $\frac{\partial u(x,t)}{\partial x}$ with dominant error term $\frac{h^3}{4}\frac{\partial^4 u(x,t)}{\partial x^4}$ is

$$
\begin{aligned}
\frac{\partial u(x,t)}{\partial x} &= \frac{1}{6h}\{-3u(x-h,t)+u(x,t)+3\,u(x+2h,t)-u(x+3h,t)\} \\
&+ \frac{h^3}{4}\frac{\partial^4 u(x,t)}{\partial x^4} + O(h^4) \;\; as \;\; h \to 0. \qquad (2.14)
\end{aligned}
$$

Suppose, now, that at the point $(x,t) = (x_2, t_n)$ the approximation to the first-order space derivative $\partial u(x,t)/\partial x$ is given by

$$
\begin{aligned}
6h\frac{\partial u(x,t)}{\partial x} &= a\,u(x-2h,t)+b\,u(x-h,t)+c\,u(x,t) \\
&+ d\,u(x+h,t)+e\,u(x+2h,t)+\frac{3}{2}h^4\frac{\partial^4 u(x,t)}{\partial x^4} \\
&+ O(h^5) \;\; as \;\; h \to 0. \qquad (2.15)
\end{aligned}
$$

Then expanding the terms $u(x-2h,t)$, $u(x-h,t)$, $u(x+h,t)$ and $u(x+2h,t)$ as Taylor series about the point (x,t) gives

$$\begin{aligned} 6h\frac{\partial u(x,t)}{\partial x} &= (a+b+c+d+e)\,u(x,t) \\ &+ (-2a-b+d+2e)\,h\frac{\partial u(x,t)}{\partial x} \\ &+ \frac{1}{2!}(4a+b+d+4e)\,h^2\frac{\partial^2 u(x,t)}{\partial x^2} \\ &+ \frac{1}{3!}(-8a-b+d+8e)\,h^3\frac{\partial^3 u(x,t)}{\partial x^3} \\ &+ \frac{1}{4!}(16a+b+d+16e+36)\,h^4\frac{\partial^4 u(x,t)}{\partial x^4} \\ &+ O(h^5) \;\; as \;\; h \to 0 \end{aligned} \qquad (2.16)$$

and equating the powers of $h^i (i = 0, 1, 2, 3, 4)$ in (2.16) gives

$$\begin{aligned} a+b+c+d+e+f &= 0, \\ -2a-b+d+2e &= 6, \\ 4a+b+d+4e &= 0, \\ -8a-b+d+8e &= 0, \\ 16a+b+16c+d+16e &= -36. \end{aligned} \qquad (2.17)$$

The solution of the linear system (2.17) is

$$a=-1, \quad b=2, \quad c=-9, \quad d=10, \quad e=-2. \qquad (2.18)$$

Hence, at the mesh point (x_2, t_n), the approximation to $\partial u(x,t)/\partial x$ is

$$\begin{aligned} \frac{\partial u(x,t)}{\partial x} &= \frac{1}{6h}\{-u(x-2h,t)+2u(x-h,t)-9u(x,t)+10u(x+h,t) \\ &- 2u(x+2h,t)\} + \frac{h^3}{4}\frac{\partial^4 u(x,t)}{\partial x^4} + O(h^4) \;\; as \;\; h \to 0. \end{aligned} \qquad (2.19)$$

Applying (2.2) with (2.9), (2.14) and (2.19) as appropriate to the N mesh points of the grid at time level $t = t_n$ leads to the system of first-order ordinary differential equations given in vector-matrix form by

$$\frac{d\mathbf{U}(t)}{dt} = -\lambda A\mathbf{U}(t) + \mathbf{b}(t), \quad t > 0 \tag{2.20}$$

with initial distribution

$$\mathbf{U}(0) = \mathbf{g} \tag{2.21}$$

in which $\mathbf{U}(t) = [U_1(t), \ldots, U_N(t)]^T$, $\mathbf{b}(t) = \frac{\lambda}{6h}[3f(t), f(t), 2f(t), 0, \ldots, 0]^T$ $\mathbf{g} = [g(x_1), g(x_2), \ldots, g(x_N)]^T$, T denoting transpose and

$$A = \frac{1}{6h}\begin{bmatrix} 1 & 0 & 3 & -1 & & & \bigcirc \\ 2 & -9 & 10 & -2 & & & \\ 9 & -18 & 11 & & & & \\ -2 & 9 & -18 & 11 & & & \\ & -2 & 9 & -18 & 11 & & \\ & & \ddots & \ddots & \ddots & \ddots & \\ \bigcirc & & & -2 & 9 & -18 & 11 \end{bmatrix}_{N\times N} \tag{2.22}$$

Solving (2.20) subject to (2.21) gives the solution

$$\mathbf{U}(t) = exp(-\lambda tA)\mathbf{U}(0) + \int_0^t exp[-\lambda A(t-s)]\mathbf{b}(s)ds \tag{2.23}$$

which satisfies the recurrence relation

$$\mathbf{U}(t+l) = exp(-\lambda lA)\mathbf{U}(t) + \int_t^{t+l} exp[-\lambda A(t+l-s)]\mathbf{b}(s)ds. \tag{2.24}$$

Approximating the matrix exponential function $exp(-\lambda lA)$ in (2.24) by

$$exp(-\lambda lA) = D^{-1}N \tag{2.25}$$

where

$$D = [I + a_1\lambda lA + a_2\lambda^2 l^2 A^2 + (\frac{1}{6} - \frac{1}{2}a_1 + a_2)\lambda^3 l^3 A^3] \tag{2.26}$$

is non-singular and

$$N = [I - (1-a_1)\lambda lA + (\frac{1}{2} - a_1 + a_2)\lambda^2 l^2 A^2] \tag{2.27}$$

which is analogous to (1.1) and the integral term by

$$\int_t^{t+l} exp(-\lambda(t+l-s)A)\mathbf{b}(s)ds = W_1\mathbf{b}(s_1) + W_2\mathbf{b}(s_2) + W_3\mathbf{b}(s_3) \quad (2.28)$$

where $s_1 \neq s_2 \neq s_3$ and W_1, W_2 and W_3 are matrices, it can be shown that

(i) <u>when $\mathbf{b}(s) = [1,1,1,\ldots,1]^T$</u>

$$W_1 + W_2 + W_3 = M_1 \quad (2.29)$$

where

$$M_1 = -(\lambda A)^{-1}(exp(-\lambda l A) - I), \quad (2.30)$$

(ii) <u>when $\mathbf{b}(s) = [s,s,s,\ldots,s]^T$</u>

$$s_1W_1 + s_2W_2 + s_3W_3 = M_2 \quad (2.31)$$

where

$$M_2 = -(\lambda A)^{-1}\left\{t\, exp(-\lambda l A) - (t+l)\,I - (\lambda A)^{-1}(exp(-\lambda l A) - I)\right\} \quad (2.32)$$

and

(iii) <u>when $\mathbf{b}(s) = [s^2, s^2, \ldots, s^2]^T$</u>

$$s_1^2W_1 + s_2^2W_2 + s_3^2W_3 = M_3 \quad (2.33)$$

where

$$\begin{aligned} M_3 &= -(\lambda A)^{-1}\left\{t^2 exp(-\lambda l A) - (t+l)^2 I - 2(\lambda A)^{-1}\{t\, exp(lA) - (t+l)\,I\right. \\ &- \left.(\lambda A)^{-1}(exp(-\lambda l A) - I)\}\right\}. \end{aligned} \quad (2.34)$$

Solving (2.29), (2.31) and (2.33) simultaneously gives

$$W_1 = \frac{s_3 - s_2}{(s_1-s_2)(s_2-s_3)(s_3-s_1)}\{s_2s_3M_1 - (s_2+s_3)M_2 + M_3\}, \quad (2.35)$$

$$W_2 = \frac{s_1 - s_3}{(s_1 - s_2)(s_2 - s_3)(s_3 - s_1)} \{s_1 s_3 M_1 - (s_1 + s_3) M_2 + M_3\} \quad (2.36)$$

and

$$W_3 = \frac{s_2 - s_1}{(s_1 - s_2)(s_2 - s_3)(s_3 - s_1)} \{s_1 s_2 M_1 - (s_1 + s_2) M_2 + M_3\}, \quad (2.37)$$

or

$$W_1 = \frac{-1}{(s_1 - s_2)(s_3 - s_1)} \{s_2 s_3 M_1 - (s_2 + s_3) M_2 + M_3\}, \quad (2.38)$$

$$W_2 = \frac{-1}{(s_1 - s_2)(s_2 - s_3)} \{s_1 s_3 M_1 - (s_2 + s_3) M_2 + M_3\} \quad (2.39)$$

and

$$W_3 = \frac{-1}{(s_2 - s_3)(s_3 - s_1)} \{s_1 s_2 M_1 - (s_2 + s_3) M_2 + M_3\}. \quad (2.40)$$

Taking $s_1 = t$, $s_2 = t + \frac{l}{2}$ and $s_3 = t + l$ gives

$$W_1 = \frac{2}{l^2} \left\{ (t^2 + \frac{3}{2} lt + \frac{l^2}{2}) M_1 - (2t + \frac{3}{2} l) M_2 + M_3 \right\}, \quad (2.41)$$

$$W_2 = \frac{-4}{l^2} \left\{ (t^2 + lt) M_1 - (2t + l) M_2 + M_3 \right\}, \quad (2.42)$$

$$W_3 = \frac{2}{l^2} \left\{ (t^2 + \frac{l}{2} t) M_1 - (2t + \frac{l}{2}) M_2 + M_3 \right\}. \quad (2.43)$$

Using (2.30), (2.32) and (2.34) in (2.41), (2.42) and (2.43) gives

$$\begin{aligned} W_1 &= \frac{2}{l^2} \Big[(t^2 + \frac{3}{2} lt + \frac{l^2}{2})(-\lambda A)^{-1}(exp(-\lambda l A) - I) \\ &- (2t + \frac{3}{2} l)(-\lambda A)^{-1} \left\{ t\, exp(-\lambda l A) - (t + l)\, I - (\lambda A)^{-1}(exp(-\lambda l A) - I) \right\} \\ &- (\lambda A)^{-1} \Big\{ t^2 exp(-\lambda l A) - (t + l)^2 I - 2(\lambda A)^{-1} \{ t\, exp(-\lambda l A) - (t + l)\, I \\ &- (\lambda A)^{-1}(exp(-\lambda l A) - I) \} \Big\} \Big], \end{aligned} \quad (2.44)$$

$$\begin{aligned} W_2 &= \frac{-4}{l^2} \Big[(t^2 + lt)(-\lambda A)^{-1}(exp(-\lambda l A) - I) \\ &+ (2t + l)(\lambda A)^{-1} \left\{ t\, exp(-\lambda l A) - (t + l)\, I - (\lambda A)^{-1}(exp(-\lambda l A) - I) \right\} \\ &- (\lambda A)^{-1} \Big\{ t^2 exp(-\lambda l A) - (t + l)^2 I - 2(\lambda A)^{-1} \{ t\, exp(-\lambda l A) - (t + l)\, I \\ &- (\lambda A)^{-1}(exp(-\lambda l A) - I) \} \Big\} \Big] \end{aligned} \quad (2.45)$$

and

$$
\begin{aligned}
W_3 &= \frac{2}{l^2}\Big[(t^2+\frac{l}{2}t+\frac{l^2}{2})(-\lambda A)^{-1}(exp(-\lambda lA)-I) \\
&+ (2t+\frac{l}{2})(\lambda A)^{-1}\Big\{t\,exp(-\lambda lA)-(t+l)\,I-(\lambda A)^{-1}(exp(-\lambda lA)-I)\Big\} \\
&- (\lambda A)^{-1}\Big\{t^2 exp(-\lambda lA)-(t+l)^2 I-2(\lambda A)^{-1}\{t\,exp(-\lambda lA)-(t+l)\,I \\
&- (\lambda A)^{-1}(exp(-\lambda lA)-I)\}\Big\}\Big] \qquad (2.\ 46)
\end{aligned}
$$

or

$$
\begin{aligned}
W_1 &= \frac{2}{l^2}((\lambda A)^{-1})^3\Big[-(t^2+\frac{3}{2}lt+\frac{l^2}{2})(\lambda A)^2(exp(-\lambda lA)-I) \\
&+ (2t+\frac{3}{2}l)(\lambda A)^2\Big\{t\,exp(-\lambda lA)-(t+l)\,I-(\lambda A)^{-1}(exp(-\lambda lA)-I)\Big\} \\
&- (\lambda A)^2\Big\{t^2 exp(lA)-(t+l)^2 I-2(\lambda A)^{-1}\{t\,exp(-\lambda lA)-(t+l)\,I \\
&- (\lambda A)^{-1}(exp(-\lambda lA)-I)\}\Big\}\Big], \qquad (2.\ 47)
\end{aligned}
$$

$$
\begin{aligned}
W_2 &= \frac{-4}{l^2}((\lambda A)^{-1})^3\Big[-(t^2+lt)(\lambda A)^2(exp(-\lambda lA)-I) \\
&+ (2t+l)(\lambda A)^2\Big\{t\,exp(-\lambda lA)-(t+l)\,I-(\lambda A)^{-1}(exp(-\lambda lA)-I)\Big\} \\
&- (\lambda A)^2\Big\{t^2 exp(lA)-(t+l)^2 I-2(\lambda A)^{-1}\{t\,exp(-\lambda lA)-(t+l)\,I \\
&- (\lambda A)^{-1}(exp(-\lambda lA)-I)\}\Big\}\Big] \qquad (2.\ 48)
\end{aligned}
$$

and

$$
\begin{aligned}
W_3 &= \frac{2}{l^2}(A^{-1})^3\Big[-(t^2+\frac{l}{2}t+\frac{l^2}{2})A^2(exp(lA)-I) \\
&+ (2t+\frac{l}{2})(\lambda A)^2\Big\{t\,exp(-\lambda lA)-(t+l)\,I-(\lambda A)^{-1}(exp(-\lambda lA)-I)\Big\} \\
&- (\lambda A)^2\Big\{t^2 exp(lA)-(t+l)^2 I-2(\lambda A)^{-1}\{t\,exp(-\lambda lA)-(t+l)\,I \\
&- \lambda A)^{-1}(exp(-\lambda lA)-I)\}\Big\}\Big]. \qquad (2.\ 49)
\end{aligned}
$$

Then it is easy to show that

$$
W_1 = \frac{2}{l^2}((\lambda A)^{-1})^3\Big\{-(\frac{\lambda^2 l^2}{2}A^2+\frac{3\lambda l}{2}A+2I)\,exp(-\lambda lA)
$$

$$+ \quad (\frac{\lambda l}{2}A + 2I)\Big\}, \qquad (2.50)$$

$$W_2 = -\frac{4}{l^2}((\lambda A)^{-1})^3\{(2I + \lambda l A)\,exp(-\lambda l A)$$

$$+ \quad (2I - \lambda l A)\}, \qquad (2.51)$$

$$W_3 = \frac{2}{l^2}((\lambda A)^{-1})^3\Big\{-(2I + \frac{\lambda l}{2}A)exp(-\lambda l A)$$

$$+ \quad (2I - \frac{3\lambda l}{2}A + \frac{\lambda^2 l^2}{2}A^2)\Big\}. \qquad (2.52)$$

Using (2.25) in (2.50)-(2.52) gives

$$W_1 = \frac{l}{6}\{(I - (4 - 9a_1 + 12a_2)\lambda l A\}\,D^{-1}, \qquad (2.53)$$

$$W_2 = \frac{2l}{3}\{(I + (1 - 3a_1 + 6a_2)\lambda l A\}\,D^{-1} \qquad (2.54)$$

and

$$W_3 = \frac{l}{6}\{(I - (3 - 9a_1 + 12a_2)\lambda l A + (1 - 3a_1 + 6a_2)\lambda^2 l^2 A^2\}\,D^{-1}. \qquad (2.55)$$

Hence (2.24) can be written as

$$\mathbf{U}(t + l) = exp(-\lambda l A)\mathbf{U}(t) + W_1\mathbf{b}(t) + W_2\mathbf{b}(t + \frac{l}{2}) + W_3\mathbf{b}(t + l). \qquad (2.56)$$

2.4 Algorithm

Assuming that r_1, r_2 and r_3 are the real zeros of

$$q(\theta) = 1 + a_1\theta + a_2\theta^2 + (\frac{1}{6} - \frac{a_1}{2} + a_2)\theta^3 \qquad (2.57)$$

then D given by (2.26) can be factorized as

$$D = (I - \frac{\lambda l}{r_1}A)(I - \frac{\lambda l}{r_2}A)(I - \frac{\lambda l}{r_3}A) \qquad (2.58)$$

and then (2.56) can be written in partial fraction form as

$$\begin{aligned}
\mathbf{U}(t+l) &= \left\{c_{11}(I-\frac{\lambda l}{r_1}A)^{-1}+c_{12}(I-\frac{\lambda l}{r_2}A)^{-1}+c_{13}(I-\frac{\lambda l}{r_3}A)^{-1}\right\}\mathbf{U}(t)\\
&+\frac{l}{6}\left\{c_{21}(I-\frac{\lambda l}{r_1}A)^{-1}+c_{22}(I-\frac{\lambda l}{r_2}A)^{-1}+c_{23}(I-\frac{\lambda l}{r_3}A)^{-1}\right\}\mathbf{b}(t)\\
&+\frac{2l}{3}\left\{c_{31}(I-\frac{\lambda l}{r_1}A)^{-1}+c_{32}(I-\frac{\lambda l}{r_2}A)^{-1}+c_{33}(I-\frac{\lambda l}{r_3}A)^{-1}\right\}\mathbf{b}(t+\frac{l}{2})\\
&+\frac{l}{6}\left\{c_{41}(I-\frac{\lambda l}{r_1}A)^{-1}+c_{42}(I-\frac{\lambda l}{r_2}A)^{-1}+c_{43}(I-\frac{\lambda l}{r_3}A)^{-1}\right\}\mathbf{b}(t+l)
\end{aligned} \tag{2.59}$$

where

$$c_{1j}=\frac{1-(1-a_1)r_j+(\frac{1}{2}-a_1+a_2)r_j^2}{\prod_{\substack{i=1\\ i\neq j}}^{3}(1-\frac{r_j}{r_i})},\quad j=1,2,3,$$

$$c_{2j}=\frac{1-(4-9a_1+12a_2)r_j}{\prod_{\substack{i=1\\ i\neq j}}^{3}(1-\frac{r_j}{r_i})},\quad j=1,2,3,$$

$$c_{3j}=\frac{1+(1-3a_1+6a_2)r_j}{\prod_{\substack{i=1\\ i\neq j}}^{3}(1-\frac{r_j}{r_i})},\quad j=1,2,3$$

and

$$c_{4j}=\frac{1-(3-9a_1+12a_2)r_j+(1-3a_1+6a_2)r_j^2}{\prod_{\substack{i=1\\ i\neq j}}^{3}(1-\frac{r_j}{r_i})},\quad j=1,2,3.$$

so that

$$\begin{aligned}
\mathbf{U}(t+l) &= A_1^{-1}\{c_{11}\mathbf{U}(t)+\frac{l}{6}(c_{21}\mathbf{b}(t)+4c_{31}\mathbf{b}(t+\frac{l}{2})+c_{41}\mathbf{b}(t+l))\}\\
&+ A_2^{-1}\{c_{12}\mathbf{U}(t)+\frac{l}{6}(c_{22}\mathbf{b}(t)+4c_{32}\mathbf{b}(t+\frac{l}{2})+c_{42}\mathbf{b}(t+l))\}\\
&+ A_3^{-1}\{c_{13}\mathbf{U}(t)+\frac{l}{6}(c_{23}\mathbf{b}(t)+4c_{33}\mathbf{b}(t+\frac{l}{2})+c_{43}\mathbf{b}(t+l))\},
\end{aligned} \tag{2.60}$$

where

$$A_i = I - \frac{\lambda l}{r_i} A, \quad i = 1, 2, 3, \tag{2.61}$$

or

$$\mathbf{U}(t + l) = \sum_{i=1}^{3} A_i^{-1} \mathbf{z}_i \tag{2.62}$$

where

$$\mathbf{z}_i = c_{1i}\mathbf{U}(t) + \frac{l}{6}\{c_{2i}\mathbf{b}(t) + 4c_{3i}\mathbf{b}(t + \frac{l}{2}) + c_{4i}\mathbf{b}(t + l)\}, \quad i = 1, 2, 3.$$

Let

$$A_i^{-1}\mathbf{z}_i = \mathbf{y}_i$$

then

$$\mathbf{U}(t + l) = \mathbf{y}_1 + \mathbf{y}_2 + \mathbf{y}_3 \tag{2.63}$$

in which $\mathbf{y}_1$, $\mathbf{y}_2$ and $\mathbf{y}_3$ are the solutions of the systems

$$A_i\mathbf{y}_i = \mathbf{z}_i, \quad i = 1, 2, 3. \tag{2.64}$$

respectively. This algorithm is presented in tabular form in Table 2.1.

2.5 Numerical Examples

In this section only a representative of many other methods based on (2.25) will be used. So taking

$$a_1 = \frac{65431}{50000}$$

and

$$a_2 = \frac{171151}{300000}$$

Taj and Twizell [38], which give a very small local truncation error, gives

$$r_1 = 2.18837132239, \quad r_2 = 2.33987492248, \quad r_3 = 2.35690139372$$

as the real zeros of (2.57). These values produce

$$c_{11} = -176.185066638, \quad c_{12} = 2051.11129521, \quad c_{13} = -1873.92622858,$$

$$c_{21} = -224.317807049, \quad c_{22} = 2358.75587416, \quad c_{23} = -2133.43806711,$$

$$c_{31} = -19.0008161810, \quad c_{32} = 326.498892802, \quad c_{33} = -306.498076621,$$

$$c_{41} = -182.736963963, \quad c_{42} = 1594.78928297, \quad c_{43} = -1411.05231901$$

2.5.1 Example 1

Consider the one space variable partial differential equation

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0, \quad 0 < x < 1, \quad t > 0. \qquad (2.65)$$

subject to the boundary conditions

$$u(0,t) = -sin(2k\pi t), \quad t > 0, \qquad (2.66)$$

where k is a positive integer and the initial condition

$$u(x,0) = sin(2k\pi x), \quad 0 \leq x \leq 1. \qquad (2.67)$$

This problem has theoretical solution

$$u(x,t) = sin\{2k\pi(x-t)\} \qquad (2.68)$$

(see Oliger [31]). The integer k gives the number of complete waves in the interval $0 \leq x \leq 1$. Using the algorithm developed in section 2.4 with the information given at the beginning of this section, the problem {(2.65)-(2.67)} is solved for $h = \frac{1}{640}$ and $l = \frac{1}{80}$ so that $r = 8.0 (r = \frac{l}{h})$, using $k = 2$ and 4 and compared with the results obtained by Arigu *et al.* [5] whose algorithm requires the use of complex arithmetic. The theoretical solutions and the numerical solutions for $k = 2$ and $k = 4$ at time $t = 0.5$ and t=10.0 respectively are depicted in Figure 2.1 - 2.4. In these experiments the method behaves smoothly over the whole interval $0 \leq x \leq 1$ and no contrived oscillations are observed. The apparent decay in amplitude in Figure 2.4 is due to the build-up of round-off errors. Maximum errors at time t=0.5, 1.0, 2.0, 4.0, 10.0, are given in Table 2.2.

2.5.2 Example 2

Consider again the one space variable partial differential equation

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0, \quad 0 < x < 1, \quad t > 0. \tag{2. 69}$$

subject to the boundary conditions

$$u(0,t) = e^{-t}, \quad t > 0, \tag{2. 70}$$

and the initial condition

$$u(x,0) = e^{x}, \quad 0 \leq x \leq 1. \tag{2. 71}$$

This problem has theoretical solution

$$u(x,t) = e^{x-t} \tag{2. 72}$$

(see Arigu *et al.* [5]), which decays as time increases. Using once again the algorithm developed in Section 2.4 with the information given at the beginning of this section the problem {(2.69)-(2.71)} is solved for $h = \frac{1}{80}$ and $l = \frac{1}{120}$ and compared once again with the results obtained by Arigu *et al.* [5]. In these experiments the method behaves smoothly over the whole interval $0 \leq x \leq 1$ and no contrived oscillations are observed. From Table 2.3 it is clear that accuracy of this method is much much better than the $O(h^2 + l^4)$ method of Arigu *et al.* From Table 2.4 it is also clear that the method is third-order at time t=1.0 and 10.0 because, as h and l are both successively halved, the errors decrease in magnitude by a factor of 8(approximately). Theoretical and numerical solutions at time t=1.0, 10.0 are depicted in Figure 2.5 - 2.8. Maximum errors at time t=0.5, 1.0, 2.0, 4.0 and 10.0 are given in Table 2.3.

2.6 Non-linear Problem

Consider the first-order non-linear hyperbolic partial differential equation

$$\frac{\partial u}{\partial t} + \frac{1}{2}\frac{\partial u^2}{\partial x} = 0, \quad ,0 \le x \le X, \quad t > 0 \qquad (2.73)$$

where $u = u(x,t)$, which is ubiquitous in wave theory and in quantum mechanics, with the boundary conditions

$$u(0,t) = f(t), \quad t > 0 \qquad (2.74)$$

and the initial condition

$$u(x,0) = g(x), \quad 0 \le x \le X \qquad (2.75)$$

where $g(x)$ is a given continuous function of x. There will exist a discontinuity between the initial condition and the boundary condition at the origin if

$$g(0) \ne f(0).$$

Equation (2.73) may be written as

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0, \quad 0 \le x \le X, \quad t > 0. \qquad (2.76)$$

Using the same discretization and finite-difference approximations as in the first-order linear case gives

$$\frac{d\mathbf{U}(t)}{dt} = A(\mathbf{U}(t))\mathbf{U}(t) + \mathbf{b}(t), \quad t > 0 \qquad (2.77)$$

with initial distribution

$$\mathbf{U}(0) = \mathbf{g} \qquad (2.78)$$

in which

$$\begin{aligned} \mathbf{U}(t) &= [U_1(t), \ldots, U_N(t)]^T, \\ \mathbf{b}(t) &= \frac{1}{6h}[3U_1(t)f(t), U_2(t)f(t), 2U_3(t)f(t), 0, \ldots, 0]^T \\ \mathbf{g} &= [g(x_1), g(x_2), \ldots, g(x_N)]^T, \end{aligned}$$

T denoting transpose and

$$A = A(\mathbf{U}(t)) = \frac{1}{6h}\begin{bmatrix} -U_1(t) & 0 & -3U_1(t) & U_1(t) & \bigcirc \\ -2U_2(t) & 9U_2(t) & -10U_2(t) & 2U_2(t) & \\ -9U_3(t) & 18U_3(t) & -11U_3(t) & & \\ 2U_4(t) & -9U_4(t) & 18U_4(t) & -11U_4(t) & \\ \ddots & \ddots & \ddots & \ddots & \\ \bigcirc & 2U_N(t) & -9U_N(t) & 18U_N(t) & -11U_N(t) \end{bmatrix}_{N\times N} \qquad (2.79)$$

Regarding this non-linear problem Algorithm 1 is modified and is given in tabular form as Algorithm 2 in Table 2.5.

By way of example, consider the problem

$$\frac{\partial u}{\partial t} + \frac{\partial(\frac{1}{2}u^2)}{\partial x} = 0, \quad ,0 \le x \le 1, \quad t > 0 \qquad (2.80)$$

or

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0, \quad ,0 \le x \le 1, \quad t > 0 \qquad (2.81)$$

with the boundary condition

$$u(0,t) = 0, \quad t > 0 \qquad (2.82)$$

and the initial condition

$$u(x,0) = x, \quad 0 \leq x \leq 1 \tag{2. 83}$$

which has theoretical solution

$$u(x,t) = \frac{x}{1+t}, \tag{2. 84}$$

(see [17]). Using Algorithm 2 the problem $\{(2.81)–(2.83)\}$ is solved for $h = \frac{1}{10}$ and $r = 1.0, 2.0$, using 150, 300 and 600 time-steps and compared with the results of the Lax-Wendroff $O(h^2 + l^3)$ method [17]. In these experiments the method behaves smoothly over the whole interval $0 \leq x \leq 1$ and no contrived oscillations are observed. The theoretical solution and the numerical solution at time $t = 15.0$ are depicted in Figure 2.9 and Figure 2.10 respectively. Maximum errors which occured at $x = 1.0$ are given in Table 2.6.

Table 2.1: Algorithm 1

Steps	Processor 1	Processor 2	Processor 3
1 Input	$l, r_1, \mathbf{U}_0, A$ $c_{11}, c_{21}, c_{31}, c_{41}$	$l, r_2, \mathbf{U}_0, A$ $c_{12}, c_{22}, c_{32}, c_{42}$	$l, r_3, \mathbf{U}_0, A$ $c_{13}, c_{23}, c_{33}, c_{43}$
2 Compute	$I - \frac{\lambda l}{r_1} A$	$I - \frac{\lambda l}{r_2} A$	$I - \frac{\lambda l}{r_3} A$
3 Decompose	$I - \frac{\lambda l}{r_1} A$ $= L_1 U_1$	$I - \frac{\lambda l}{r_2} A$ $= L_2 U_2$	$I - \frac{\lambda l}{r_3} A$ $= L_3 U_3$
4 Evaluate	$\mathbf{b}(t)$, $\mathbf{b}(t + \frac{l}{2})$ $\mathbf{b}(t + l)$	$\mathbf{b}(t)$, $\mathbf{b}(t + \frac{l}{2})$ $\mathbf{b}(t + l)$	$\mathbf{b}(t)$, $\mathbf{b}(t + \frac{l}{2})$ $\mathbf{b}(t + l)$
5 Using	$\mathbf{w}_1(t) = \frac{l}{6}(c_{21}\mathbf{b}(t)$ $+4c_{31}\mathbf{b}(t + \frac{l}{2})$ $+c_{41}\mathbf{b}(t + l))$	$\mathbf{w}_2(t) = \frac{l}{6}(c_{22}\mathbf{b}(t)$ $+4c_{32}\mathbf{b}(t + \frac{l}{2})$ $+c_{42}\mathbf{b}(t + l))$	$\mathbf{w}_3(t) = \frac{l}{6}(c_{23}\mathbf{b}(t)$ $+4c_{33}\mathbf{b}(t + \frac{l}{2})$ $+c_{43}\mathbf{b}(t + l))$
6 Solve	$L_1 U_1 \mathbf{y}_1(t)$ $= c_{11}\mathbf{U}(t) + \mathbf{w}_1(t)$	$L_2 U_2 \mathbf{y}_2(t)$ $= c_{12}\mathbf{U}(t) + \mathbf{w}_2(t)$	$L_3 U_3 \mathbf{y}_3(t)$ $= c_{13}\mathbf{U}(t) + \mathbf{w}_3(t)$
7	$\mathbf{U}(t + l) = \mathbf{y}_1(t) + \mathbf{y}_2(t) + \mathbf{y}_3(t)$		
8	GO TO Step 4 for next time step		

Table 2.2: Maximum errors for Example 1 at $t = 0.5, 1.0, 2.0, 4.0, 10$

t	0.5	1.0	2.0	4.0	10.0
k=2	-0.616D-3	-0.110D-2	-0.110D-2	-0.110D-2	-0.110D-2
*	0.271D-2	0.269D-1	0.261D-1	0.260D-2	—
k=4	-0.962D-2	-0.181D-1	-0.181D-1	-0.181D-1	-0.181D-1
*	—	—	—	—	0.641D-1

* Maximum absolute errors of Arigu *et al.*[5] $O(h^2 + l^3)$ Method

Table 2.3: Maximum errors for Example 2 at $t = 0.5, 1.0, 2.0, 4.0, 10.0$

t	0.5	1.0	2.0	4.0	10.0
	-0.394D-6	-0.450D-6	-0.165D-6	-0.224D-7	-0.555D-10
*	—	—	0.511D-2	0.215D-4	0.869D-6

* Maximum absolute errors of Arigu *et al.*[5] $O(h^2 + l^4)$ Method

Table 2.4: Maximum errors for Example 2 showing third-order accuracy.

h, l	0.1	0.05	0.025	0.0125
$t = 1.0$	-0.192D-03	-0.236D-04	-0.308D-05	-0.423D-06
$t = 10.0$	0.341D-05	0.557D-06	0.820D-07	0.112D-07

Table 2.5: Algorithm 2

Steps	Processor 1	Processor 2	Processor 3
1 Input	$l, r_1, \mathbf{U}_0$ $c_{11}, c_{21}, c_{31}, c_{41}$	$l, r_2, \mathbf{U}_0$ $c_{12}, c_{22}, c_{32}, c_{42}$	$l, r_3, \mathbf{U}_0$ $c_{13}, c_{23}, c_{33}, c_{43}$
2 Update	A	A	A
3 Compute	$I - \frac{\Delta l}{r_1}A$	$I - \frac{\Delta l}{r_2}A$	$I - \frac{\Delta l}{r_3}A$
4 Decompose	$I - \frac{\Delta l}{r_1}A$ $= L_1U_1$	$I - \frac{\Delta l}{r_2}A$ $= L_2U_2$	$I - \frac{\Delta l}{r_3}A$ $= L_3U_3$
5 Evaluate	$\mathbf{b}(t), \mathbf{b}(t+\frac{l}{2})$ $\mathbf{b}(t+l)$	$\mathbf{b}(t), \mathbf{b}(t+\frac{l}{2})$ $\mathbf{b}(t+l)$	$\mathbf{b}(t), \mathbf{b}(t+\frac{l}{2})$ $\mathbf{b}(t+l)$
6 Using	$\mathbf{w}_1(t) = \frac{l}{6}(c_{21}\mathbf{b}(t)$ $+4c_{31}\mathbf{b}(t+\frac{l}{2})$ $+c_{41}\mathbf{b}(t+l))$	$\mathbf{w}_2(t) = \frac{l}{6}(c_{22}\mathbf{b}(t)$ $+4c_{32}\mathbf{b}(t+\frac{l}{2})$ $+c_{42}\mathbf{b}(t+l))$	$\mathbf{w}_3(t) = \frac{l}{6}(c_{23}\mathbf{b}(t)$ $+4c_{33}\mathbf{b}(t+\frac{l}{2})$ $+c_{43}\mathbf{b}(t+l))$
7 Solve	$L_1U_1\mathbf{y}_1(t)$ $= c_{11}\mathbf{U}(t) + \mathbf{w}_1(t)$	$L_2U_2\mathbf{y}_2(t)$ $= c_{12}\mathbf{U}(t) + \mathbf{w}_2(t)$	$L_3U_3\mathbf{y}_3(t)$ $= c_{13}\mathbf{U}(t) + \mathbf{w}_3(t)$
8	$\mathbf{U}(t+l) = \mathbf{y}_1(t) + \mathbf{y}_2(t) + \mathbf{y}_3(t)$		
9	GO TO Step 2 for next time step		

Table 2.6: Maximum errors for non-linear problem

Time steps	h	r	Maximum absolute errors	*
150	0.1	1	0.54D-03	0.79D-03
150	0.1	2	0.36D-03	0.38D-03
300	0.1	1	0.18D-03	0.12D-02
300	0.1	2	0.11D-03	0.61D-03
600	0.1	1	0.33D-04	—
600	0.1	2	0.66D-05	—

* Maximum absolute errors of Lax-Wendroff $O(h^2 + l^3)$ Method [17](p. 426)

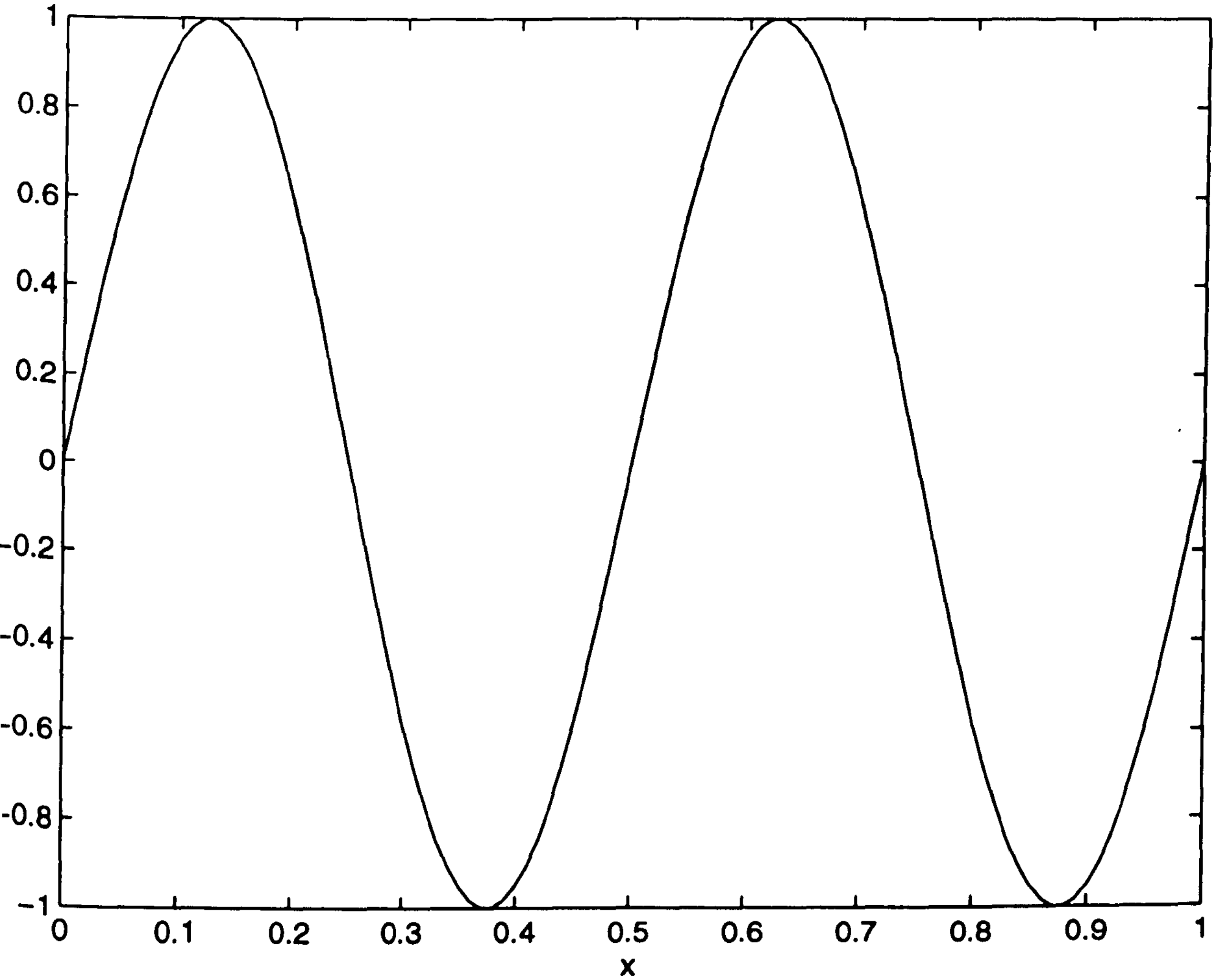

Figure 2.1: Theoretical solution of example 1 for $k = 2$ at time t=0.5

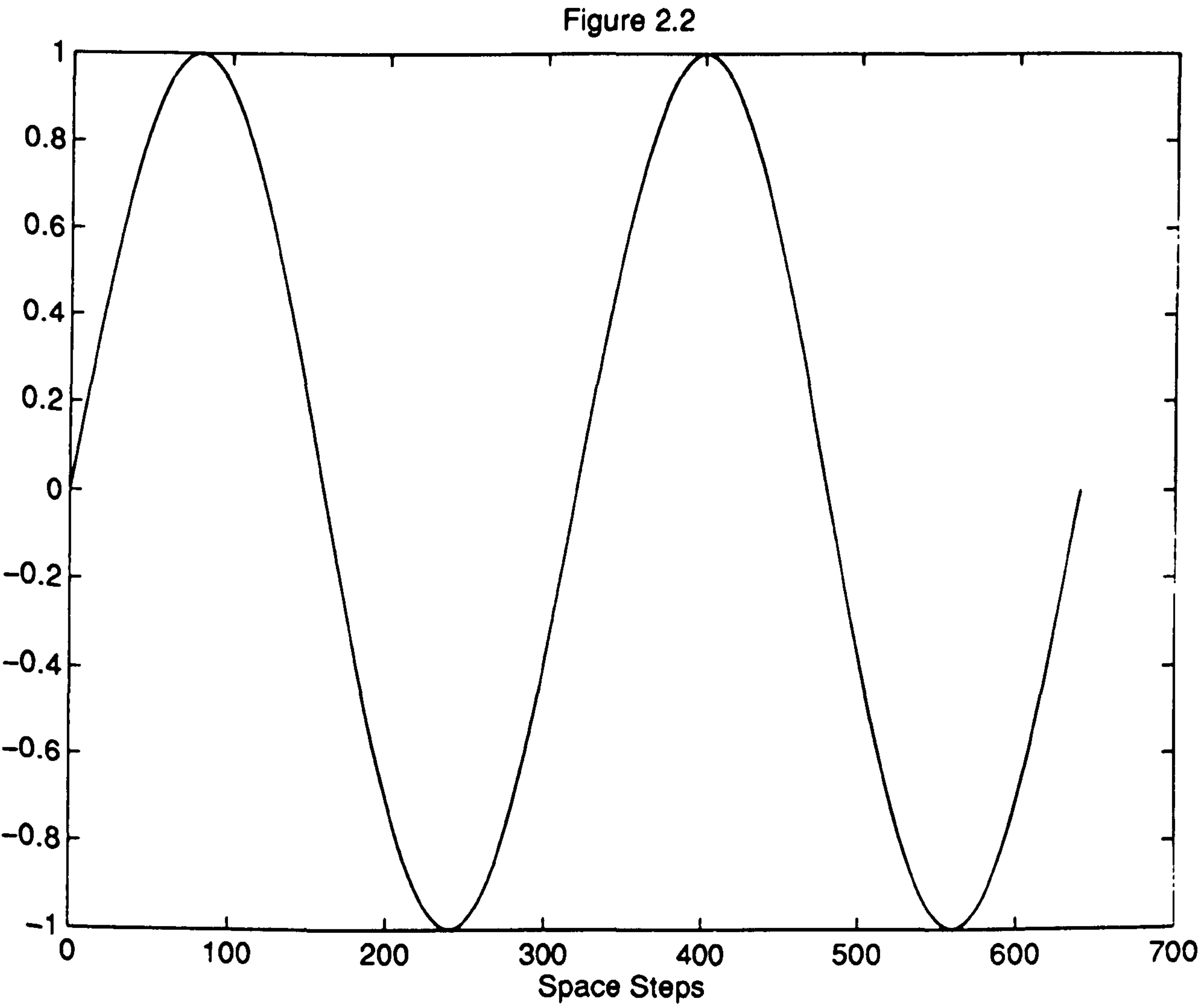

Figure 2.2: Numerical solution of example 1 for $k = 2$, $h = \frac{1}{640}$ and $l = \frac{1}{80}$ at time t=0.5

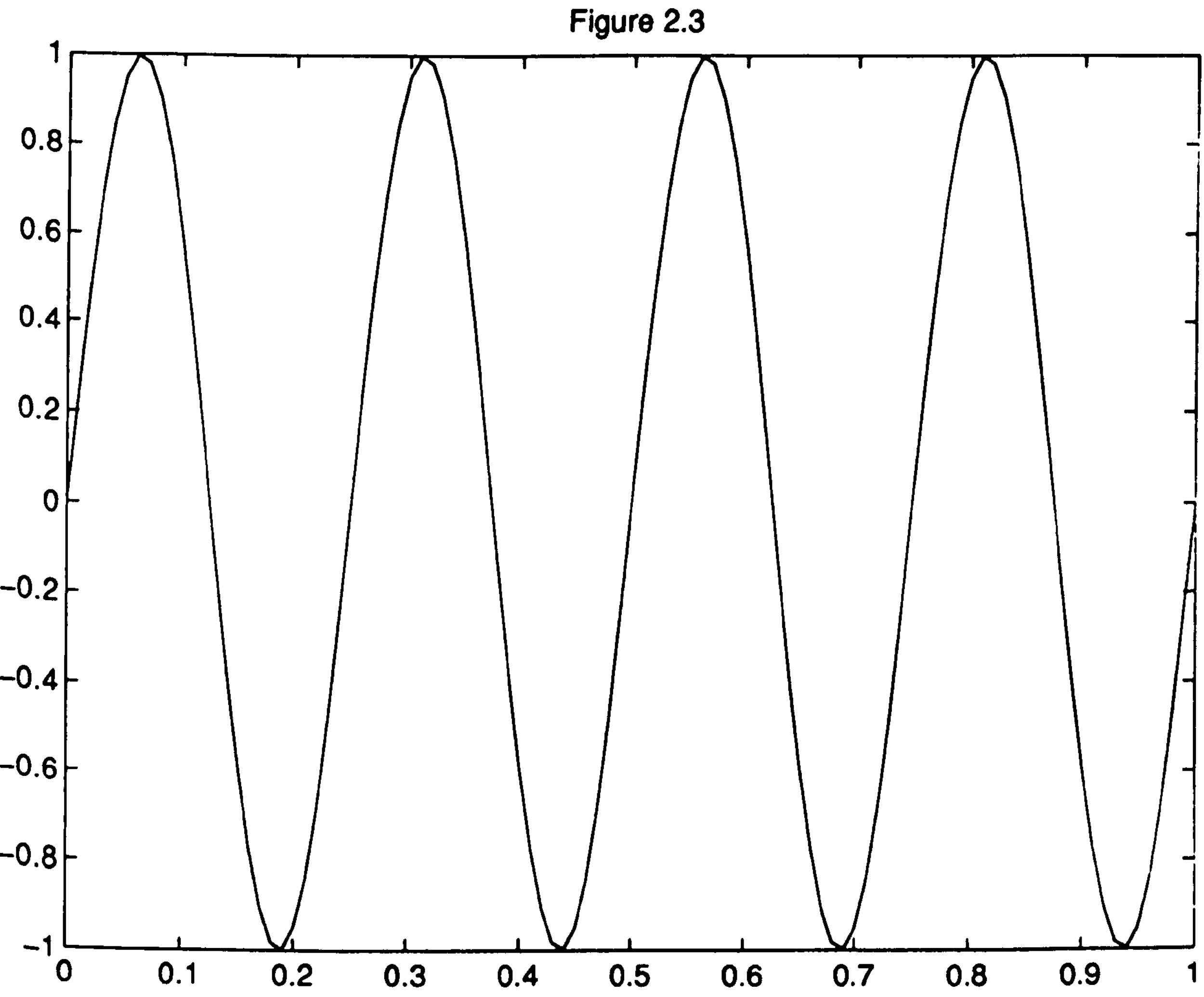

Figure 2.3: Theoretical solution of example 1 for $k = 4$ at time t=10.0

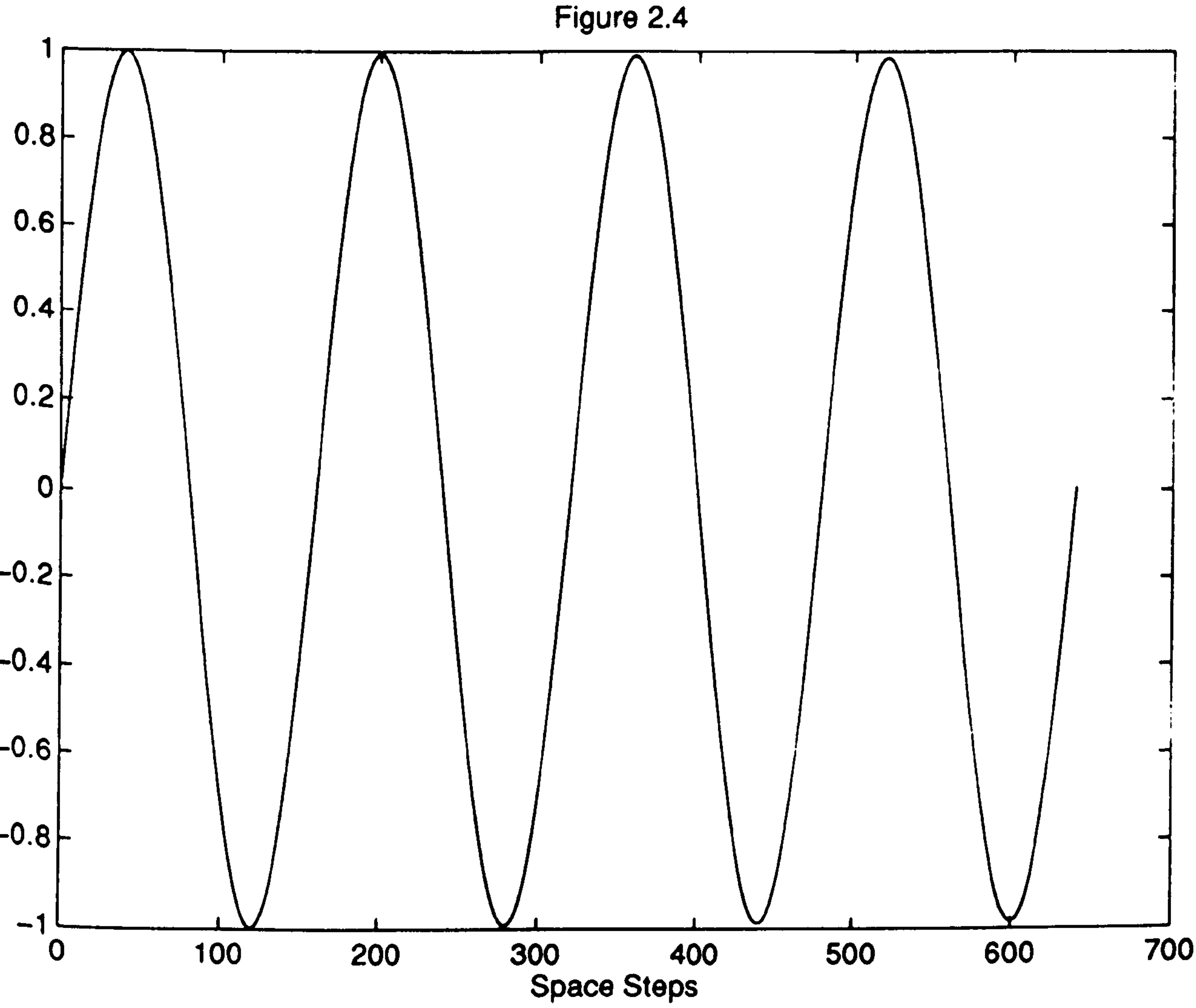

Figure 2.4: Numerical solution of example 1 for $k = 4$, $h = \frac{1}{640}$ and $l = \frac{1}{80}$ at time t=10.0

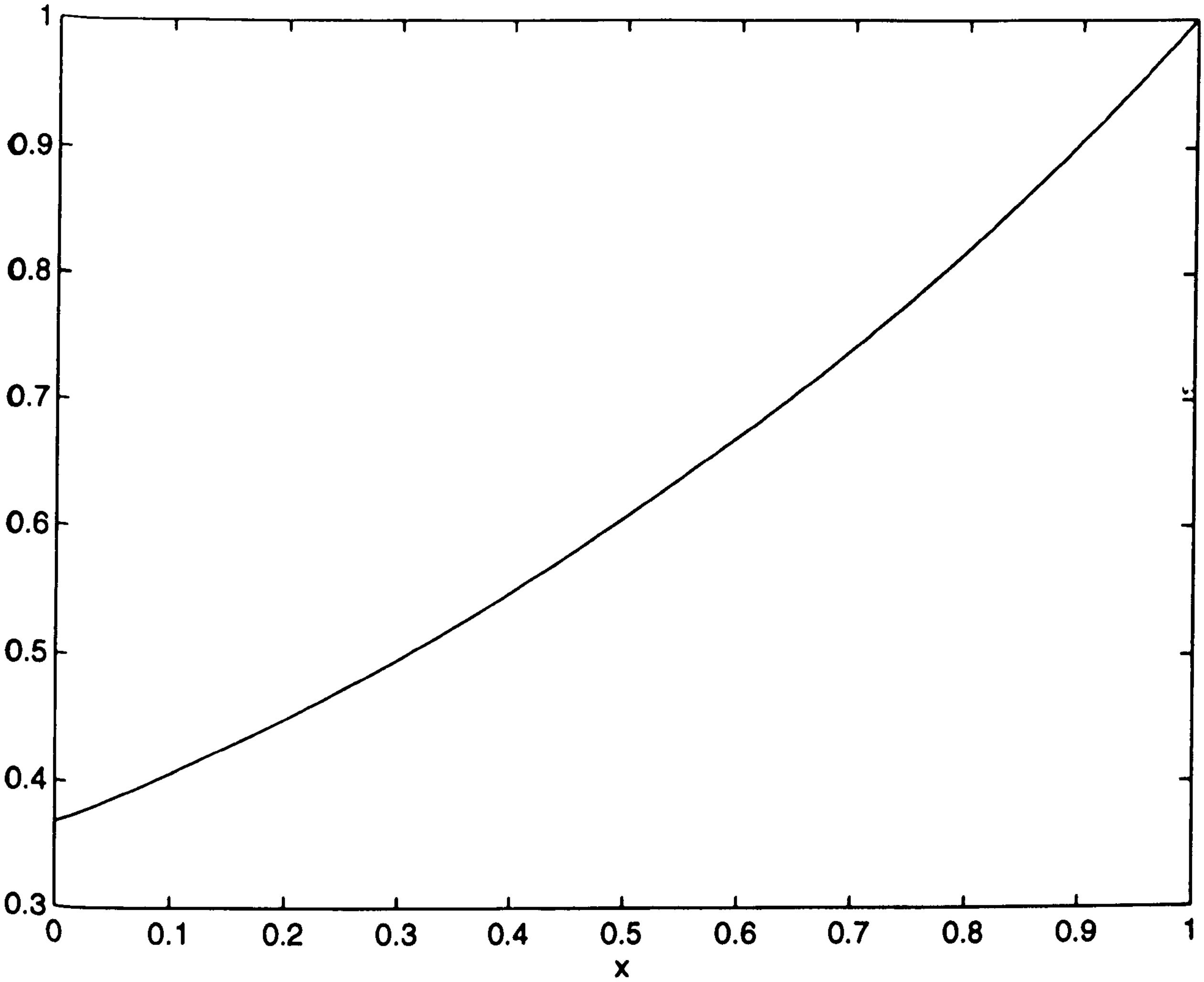

Figure 2.5: Theoretical solution of example 2 at time t=1.0

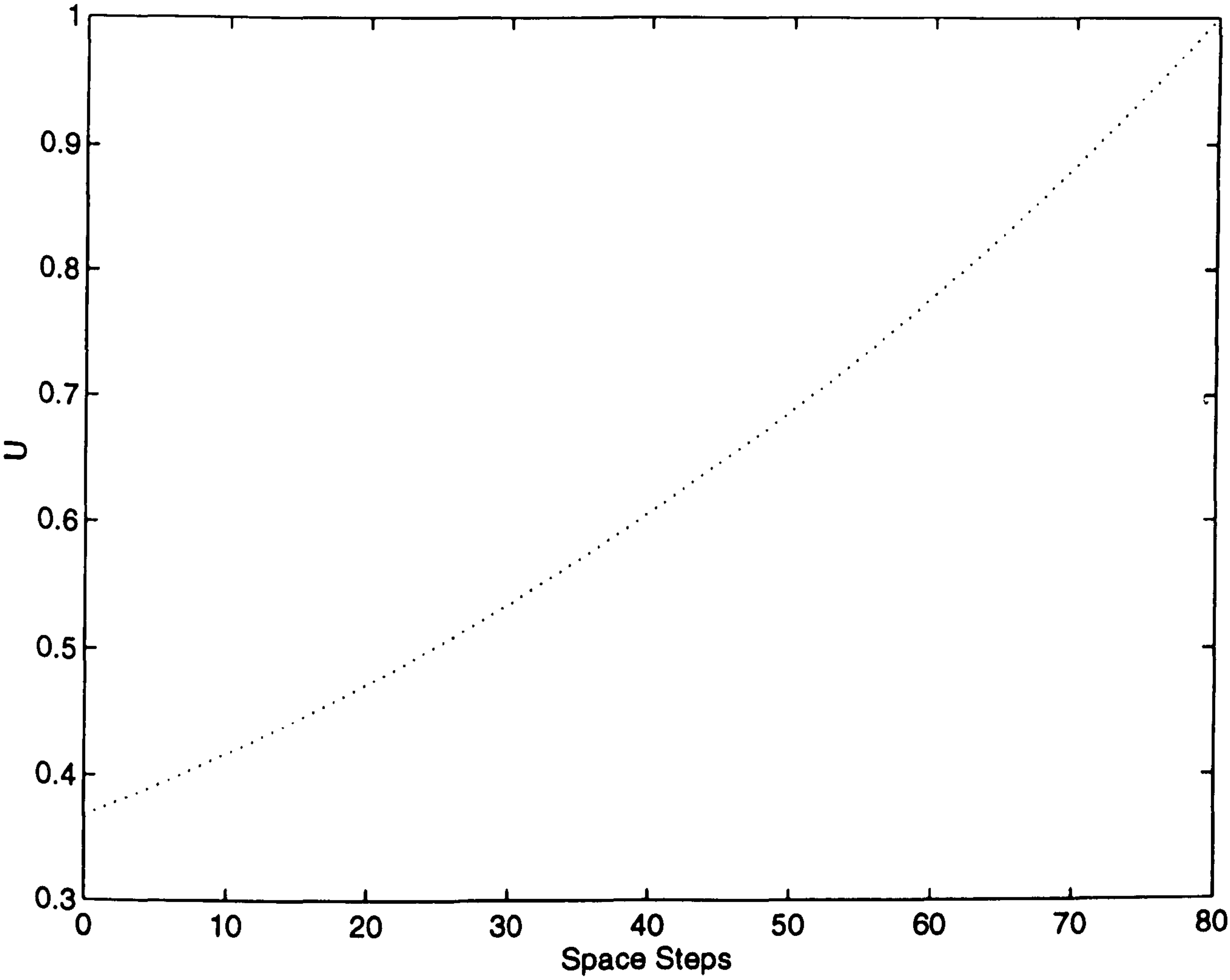

Figure 2.6: Numerical solution of example 2 for $h = \frac{1}{80}$ and $l = \frac{1}{120}$ at time t=1.0

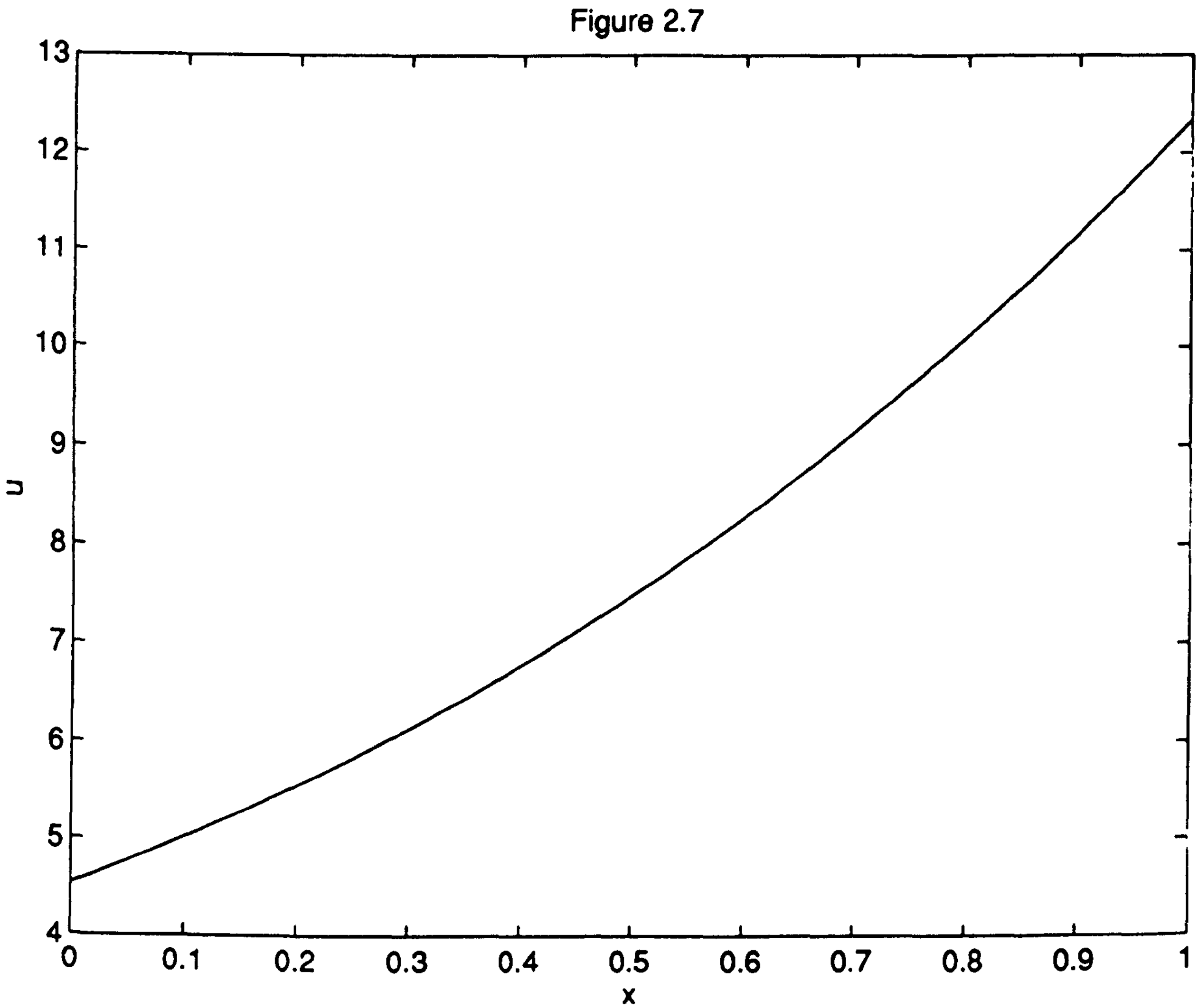

Figure 2.7: Theoretical solution of example 2 at time t=10.0

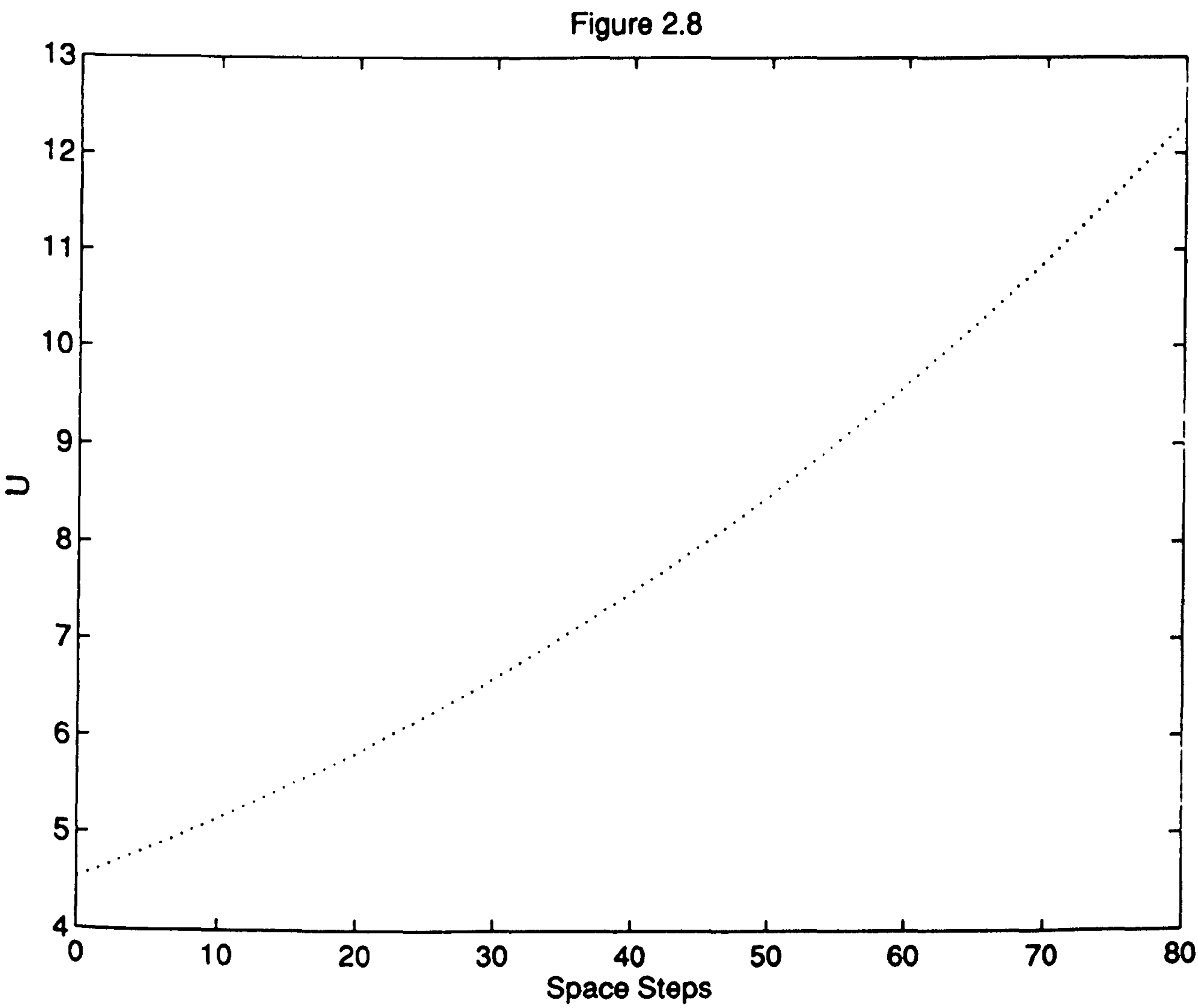

Figure 2.8: Numerical solution of example 2 for $h = \frac{1}{80}$ and $l = \frac{1}{120}$ at time t=10.0

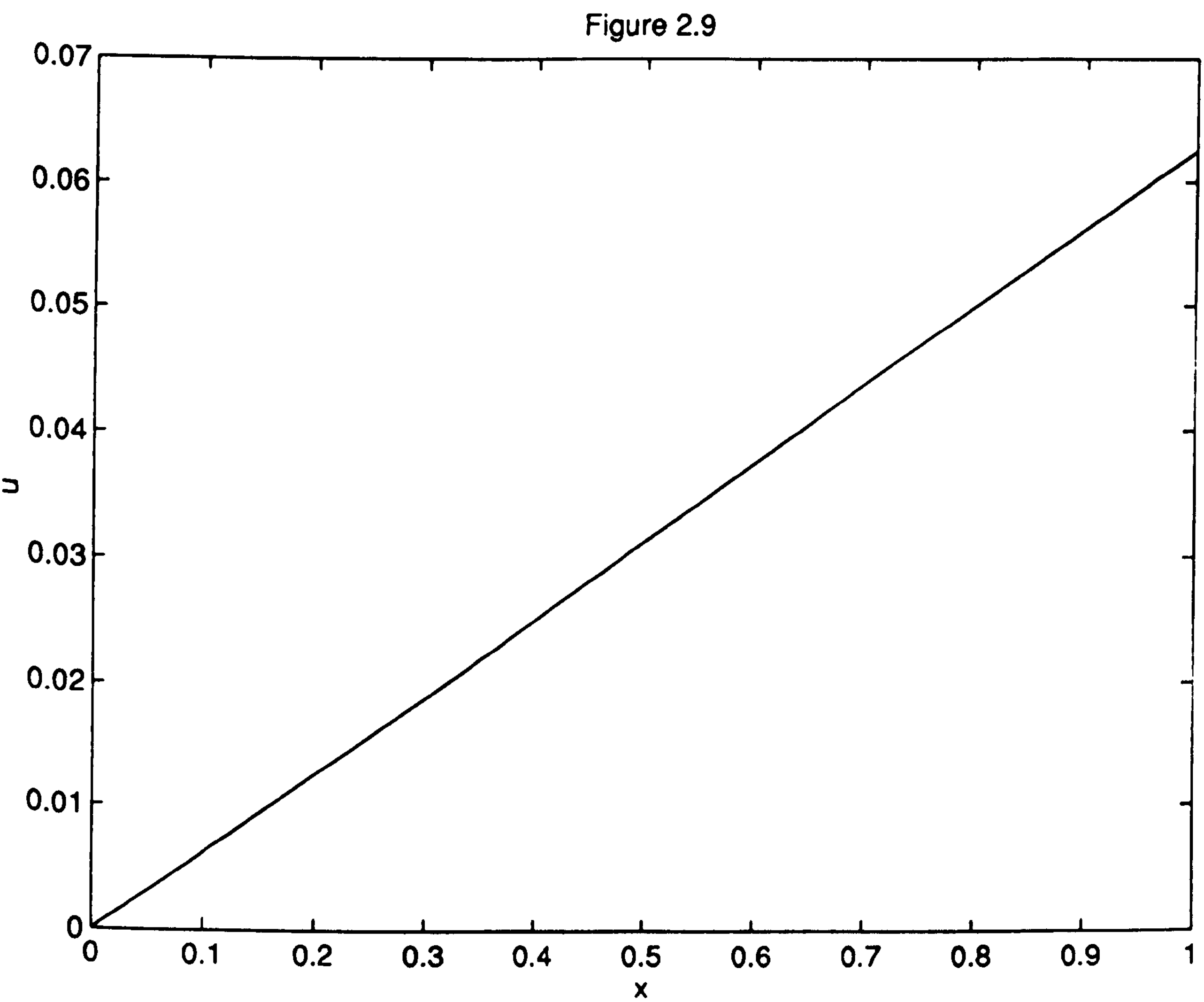

Figure 2.9: Theoretical solution of Non-Linear Problem at t=15.

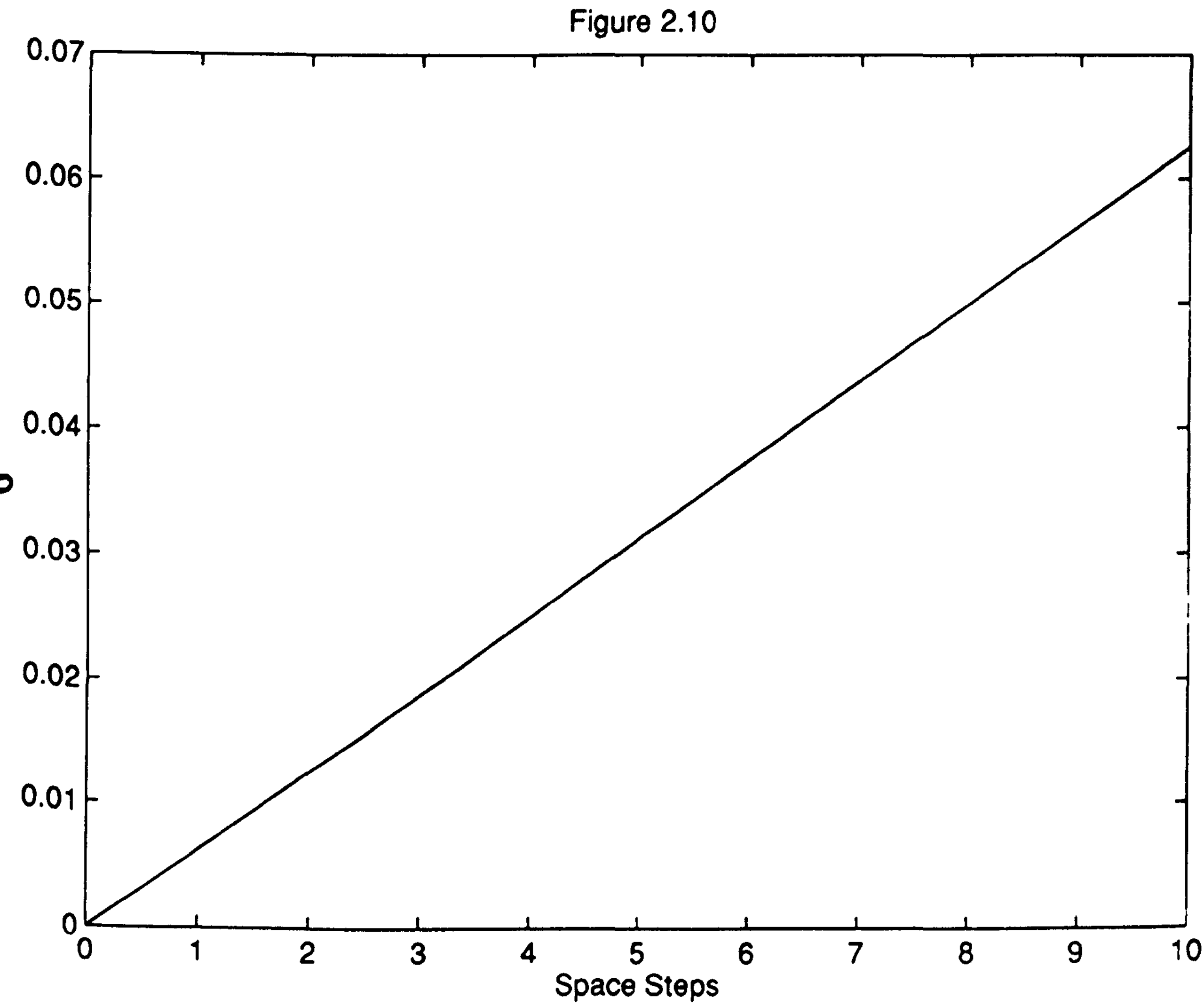

Figure 2.10: Numerical solution of Non-Linear Problem using h=0.1 and r=1.0 at t=15.

Chapter 3

Fourth-Order Numerical Methods for the Advection Equation

To develop fourth-order numerical methods for first-order hyperbolic partial differential equations of the type (2.1) with appropriate initial and boundary conditions specified, the space derivative in the partial differential equation is replaced by new fourth-order finite-difference approximations resulting in a system of first-order ordinary differential equations the solution of which satisfies a recurrence relation. The accuracy in time is controlled by a fourth-order approximation to the matrix exponential function which is introduced by Taj and Twizell [39].

3.1 The Method

Assume that the combination

$$a\,u(x-4h,t)+b\,u(x-3h,t)+c\,u(x-2h,t)+d\,u(x-h,t)+e\,u(x,t)$$

gives the fourth-order approximation to $\frac{\partial u}{\partial x}$ at (x,t). Then expanding the terms $u(x-4h,t), u(x-3h,t), u(x-2h,t)$ and $u(x-h,t)$ as Taylor series about the point (x,t) gives

$$\begin{aligned} a\,u(x-4h,t)+b\,u(x-3h,t) &+ c\,u(x-2h,t)+d\,u(x-h,t)+e\,u(x,t) \\ &= (a+b+c+d+e)u(x,t) \\ &+ (-4a-3b-2c-d)h\frac{\partial u}{\partial x} \\ &+ \frac{1}{2!}(16a+9b+4c+d)h^2\frac{\partial^2 u}{\partial x^2} \\ &+ \frac{1}{3!}(-64a-27b-8c-d)h^3\frac{\partial^3 u}{\partial x^3} \\ &+ \frac{1}{4!}(256a+81b+16c+d)h^4\frac{\partial^4 u}{\partial x^4} \\ &+ \frac{1}{5!}(-1024a-243b-32c-d)h^5\frac{\partial^5 u}{\partial x^5} \\ &+ O(h^6) \;\; as \;\; h\to 0. \end{aligned} \qquad (3.1)$$

Equating the powers of $h^i (i=0,2,3,4)$ in (3.1) to zero and the power of h to 1 gives

$$\begin{aligned} e+d+c+b+a &= 0 \\ -d-2c-3b-4a &= 1 \\ d+4c+9b+16a &= 0 \\ -d-8c-27b-64a &= 0 \\ d+16c+81b+256a &= 0. \end{aligned} \qquad (3.2)$$

The solution of this linear system is

$$a=\frac{1}{4},\quad b=\frac{-4}{3},\quad c=3,\quad d=-4,\quad e=\frac{25}{12}.$$

Thus

$$\begin{aligned} \frac{1}{4}\,u(x-4h,t) &- \frac{4}{3}u(x-3h,t)+3\,u(x-2h,t)-4\,u(x-h,t)+\frac{25}{12}\,u(x,t) \\ &= h\frac{\partial u}{\partial x}-\frac{1}{5}h^5\frac{\partial^5 u}{\partial x^5}+O(h^6) \;\; as \;\; h\to 0. \end{aligned} \qquad (3.3)$$

or

$$\frac{1}{12}\{3u(x-4h,t) - 16u(x-3h,t)+36u(x-2h,t)-48u(x-h,t)$$
$$+25u(x,t)\} = h\frac{\partial u}{\partial x}-\frac{1}{5}h^5\frac{\partial^5 u}{\partial x^5}+O(h^6) \quad as \quad h\to 0. \qquad (3.4)$$

Thus the desired approximation to $\frac{\partial u}{\partial x}$ is given by

$$\begin{aligned}\frac{\partial u}{\partial x} &= \frac{1}{12h}\{3u(x-4h,t)-16u(x-3h,t)\\ &+ 36u(x-2h,t)-48u(x-h,t)+25u(x,t)\}\\ &+ \frac{1}{5}h^4\frac{\partial^5 u}{\partial x^5}+O(h^5) \quad as \quad h\to 0. \end{aligned} \qquad (3.5)$$

Equation (3.5) is valid only for $(x,t)=(x_m,t_n)$ with $m=4,5,\ldots,N$. To attain the same accuracy at the end point (x_1,t_n), (x_2,t_n) and (x_3,t_n) special formulae must be devolped which approximate $\frac{\partial u}{\partial x}$ not only to fourth-order but also with dominant error term $\frac{1}{5}h^4\frac{\partial^5 u}{\partial x^5}$ for $x=x_1,x_2,x_3$ and $t=t_n$. Consider then the approximation to $\frac{\partial u}{\partial x}$ at the point $(x,t)=(x_1,t_n)$; let

$$\begin{aligned}12h\frac{\partial u}{\partial x} &= a\,u(x-h,t)+b\,u(x,t)+c\,u(x+h,t)+d\,u(x+2h,t)\\ &+ e\,u(x+3h,t)+f\,u(x+4h,t)+\frac{12}{5}h^5\frac{\partial^5 u}{\partial x^5}\\ &+ O(h^6) \quad as \quad h\to 0. \end{aligned} \qquad (3.6)$$

Expending the terms $u(x-h,t), u(x+h,t), u(x+2h,t), u(x+3h,t)$ and $u(x+4h,t)$ as Taylor series about the point (x,t) gives

$$\begin{aligned}12h\frac{\partial u}{\partial x} &= (a+b+c+d+e+f)u(x,t)\\ &+ (-a+c+2d+3e+4f)h\frac{\partial u}{\partial x}\\ &+ \frac{1}{2}(a+c+4d+9e+16f)h^2\frac{\partial^2 u}{\partial x^2}\\ &+ \frac{1}{6}(-a+c+8d+27e+64f)h^3\frac{\partial^3 u}{\partial x^3}\\ &+ \frac{1}{24}(a+c+16d+81e+256f)h^4\frac{\partial^4 u}{\partial x^4}\end{aligned}$$

$$+ \frac{1}{120}(-a + c + 32d + 243e + 1024f + \frac{12}{5})h^5\frac{\partial^5 u}{\partial x^5}$$
$$+ O(h^6) \quad as \quad h \to 0. \qquad (3.7)$$

Equating the powers of $h^i (i = 0, 1, 2, 3, 4, 5)$ in (3.7) gives

$$\begin{aligned}
b + a + c + d + e + f &= 0 \\
-a + c + 2d + 3e + 4f &= 12 \\
a + c + 4d + 9e + 16f &= 0 \qquad (3.8) \\
-a + c + 8d + 27e + 64f &= 0 \\
a + c + 16d + 81e + 256f &= 0 \\
-a + c + 32d + 243e + 1024f &= -288.
\end{aligned}$$

The solution of the linear system (3.8) is

$$a = 0, \quad b = -25, \quad c = 48, \quad d = -36, \quad e = 16, \quad f = -3.$$

thus

$$\begin{aligned}
\frac{\partial u(x,t)}{\partial x} &= \frac{1}{12h}\{-25u(x,t) + 48u(x+h,t) \\
&- 36u(x+2h,t) + 16u(x+3h,t) - 3u(x+4h,t)\} \\
&+ \frac{1}{5}h^4\frac{\partial^5 u}{\partial x^5} + O(h^5) \quad as \quad h \to 0. \qquad (3.9)
\end{aligned}$$

Consider, now the approximation to $\frac{\partial u(x,t)}{\partial x}$ at the point $(x,t) = (x_2, t_n)$; let

$$\begin{aligned}
12h\frac{\partial u}{\partial x} &= a\,u(x-2h,t) + b\,u(x-h,t) + c\,u(x,t) + d\,u(x+h,t) \\
&+ e\,u(x+2h,t) + f\,u(x+3h,t) + \frac{12}{5}h^5\frac{\partial^5 u}{\partial x^5} \\
&+ O(h^6) \quad as \quad h \to 0. \qquad (3.10)
\end{aligned}$$

Expending the terms $u(x-2h,t), u(x-h,t), u(x+h,t), u(x+2h,t)$ and $u(x+3h,t)$ as Taylor series about the point (x,t) gives

$$12h\frac{\partial u}{\partial x} = (a + b + c + d + e + f)u(x,t)$$

$$
\begin{aligned}
&+ \quad (-2a - b + d + 2e + 3f)h\frac{\partial u}{\partial x} \\
&+ \quad \frac{1}{2}(4a + b + d + 4e + 9f)h^2\frac{\partial^2 u}{\partial x^2} \\
&+ \quad \frac{1}{6}(-8a - b + d + 8e + 27f)h^3\frac{\partial^3 u}{\partial x^3} \\
&+ \quad \frac{1}{24}(16a + b + d + 16e + 81f)h^4\frac{\partial^4 u}{\partial x^4} \\
&+ \quad \frac{1}{120}(-32a - b + d + 32e + 243f + \frac{12}{5})h^5\frac{\partial^5 u}{\partial x^5} \\
&+ \quad O(h^6) \;\; as \;\; h \to 0. \qquad (3.11)
\end{aligned}
$$

Equating the powers of $h^i (i = 0, 1, 2, 3, 4, 5)$ in (3.11) gives the system

$$
\begin{aligned}
c + b + a + d + e + f &= 0 \\
-b - 2a + d + 2e + 3f &= 12 \\
b + 4a + d + 4e + 9f &= 0 \\
-b - 8a + d + 8e + 27f &= 0 \\
b + 16a + d + 16e + 81f &= 0 \\
-b - 32a + d + 32e + 243f &= -288
\end{aligned}
\qquad (3.12)
$$

which has solution

$$a = 3, \quad b = -18, \quad c = 20, \quad d = -12, \quad e = 9, \quad f = -2.$$

Thus

$$
\begin{aligned}
\frac{\partial u(x,t)}{\partial x} &= \frac{1}{12h}\{3u(x - 2h, t) - 18u(x - h, t) \\
&+ 20u(x,t) - 12u(x + h, t) + 9u(x + 2h, t) - 2u(x + 3h, t)\} \\
&+ \frac{1}{5}h^4\frac{\partial^5 u}{\partial x^5} + O(h^5) \;\; as \;\; h \to 0. \qquad (3.13)
\end{aligned}
$$

is the desired fourth-order approximation to $\frac{\partial u(x,t)}{\partial x}$ with dominant error term $\frac{h^4}{5}\frac{\partial^5 u(x,t)}{\partial x^5}$ at the point (x_2, t_n).

Consider, next the approximation to $\frac{\partial u(x,t)}{\partial x}$ at the point $(x,t) = (x_3, t_n)$; let

$$
\begin{aligned}
12h\frac{\partial u}{\partial x} &= a\,u(x-3h,t) + b\,u(x-2h,t) + c\,u(x-h,t) + d\,u(x,t) \\
&+ e\,u(x+h,t) + f\,u(x+2h,t) + \frac{12}{5}h^5\frac{\partial^5 u}{\partial x^5} \\
&+ O(h^6) \;\; as \;\; h \to 0. \qquad (3.\ 14)
\end{aligned}
$$

Expanding the terms $u(x-3h,t), u(x-2h,t), u(x-h,t), u(x+h,t)$ and $u(x+2h,t)$ as Taylor series about the point (x,t) gives

$$
\begin{aligned}
12h\frac{\partial u}{\partial x} &= (a+b+c+d+e+f)u(x,t) \\
&+ (-3a-2b-c+e+2f)h\frac{\partial u}{\partial x} \\
&+ \frac{1}{2}(9a+4b+c+e+4f)h^2\frac{\partial^2 u}{\partial x^2} \\
&+ \frac{1}{6}(-27a-8b-c+e+8f)h^3\frac{\partial^3 u}{\partial x^3} \\
&+ \frac{1}{24}(81a+16b+c+e+16f)h^4\frac{\partial^4 u}{\partial x^4} \\
&+ \frac{1}{120}(-243a-32b-c+e+32f+\frac{12}{5})h^5\frac{\partial^5 u}{\partial x^5} \\
&+ O(h^6) \;\; as \;\; h \to 0. \qquad (3.\ 15)
\end{aligned}
$$

Equating the powers of $h^i (i = 0,1,2,3,4,5)$ in (3.15) gives

$$
\begin{aligned}
d+e+c+b+a+f &= 0 \\
e-c-2b-3a+2f &= 12 \\
e+c+4b+9a+4f &= 0 \qquad (3.\ 16) \\
e-c-8b-27a+8f &= 0 \\
e+c+16b+81a+16f &= 0 \\
e-c-32b-243a+32f &= -288
\end{aligned}
$$

The solution of the linear system (3.16) is

$$a = 2, \quad b = -9, \quad c = 12, \quad d = -20, \quad e = 18, \quad f = -3.$$

Thus

$$\begin{aligned} \frac{\partial u(x,t)}{\partial x} &= \frac{1}{12h}\{2u(x-3h,t) - 9u(x-2h,t) \\ &+ 12u(x-h,t) - 20u(x,t) + 18u(x+h,t) - 3u(x+2h,t)\} \\ &+ \frac{1}{5}h^4\frac{\partial^5 u}{\partial x^5} + O(h^5) \ \ as \ \ h \to 0. \end{aligned} \tag{3.17}$$

is the desired approximation to $\frac{\partial u(x,t)}{\partial x}$ at the point (x_3, t_n).

Applying (2.2) with (3.5) or (3.9) or (3.13) or (3.17) as appropriate to the N mesh points at the time level $t = nl$, leads to the system of first-order ordinary differential equations given in vector-matrix form as

$$\frac{d\mathbf{U}(t)}{dt} = -\lambda A\mathbf{U}(t) + \mathbf{b}(t), \quad t > 0 \tag{3.18}$$

with initial distribution

$$\mathbf{U}(0) = \mathbf{g} \tag{3.19}$$

in which

$$\begin{aligned} \mathbf{U}(t) &= [U_1(t), \ldots, U_N(t)]^T, \\ \mathbf{b}(t) &= \tfrac{\lambda}{12h}[0, -3f(t), -2f(t), -3f(t), 0, \ldots, 0]^T, \\ \mathbf{g} &= [g(x_1), g(x_2), \ldots, g(x_N)]^T, \end{aligned}$$

T denoting transpose and

$$A = \frac{1}{12h}\begin{bmatrix} -25 & 48 & -36 & 16 & -3 & & & & \bigcirc \\ -18 & 20 & -12 & 9 & -2 & & & & \\ -9 & 12 & -20 & 18 & -3 & & & & \\ -16 & 36 & -48 & 25 & 0 & & & & \\ 3 & -16 & 36 & -48 & 25 & & & & \\ & 3 & -16 & 36 & -48 & 25 & & & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & & \\ \bigcirc & & & 3 & -16 & 36 & -48 & 25 & \end{bmatrix}_{N\times N} \tag{3.20}$$

It is observed that the matrix A has distinct eigenvalues with negative real parts for N=7, 9, 19 and 39 given in Appendix A.

Solving (3.18) subject to (3.19) gives the solution

$$\mathbf{U}(t) = exp(-\lambda t A)\mathbf{U}(0) + \int_0^t exp[-\lambda A(t-s)]\mathbf{b}(s)ds \qquad (3.21)$$

which satisfies the recurrence relation

$$\mathbf{U}(t+l) = exp(-\lambda l A)\mathbf{U}(t) + \int_t^{t+l} exp[-\lambda A(t+l-s)]\mathbf{b}(s)ds. \qquad (3.22)$$

Approximating the matrix exponential function $exp(-\lambda l A)$ in (3.22) by

$$exp(-\lambda l A) = D^{-1}N \qquad (3.23)$$

where

$$D = I + a_1\lambda l A + a_2\lambda^2 l^2 A^2 + a_3\lambda^3 l^3 A^3 + (\frac{-1}{24} + \frac{1}{6}a_1 - \frac{1}{2}a_2 + a_3)\lambda^4 l^4 A^4 \qquad (3.24)$$

is non-singular and

$$N = I - (1-a_1)\lambda l A + (\frac{1}{2} - a_1 + a_2)\lambda^2 l^2 A^2 - (\frac{1}{6} - \frac{1}{2}a_1 + a_2 - a_3)\lambda^3 l^3 A^3 \qquad (3.25)$$

which is analogous to (1.2) and the integral term by

$$\int_t^{t+l} exp(-\lambda(t+l-s)A)\mathbf{b}(s)ds = W_1\mathbf{b}(s_1) + W_2\mathbf{b}(s_2) + W_3\mathbf{b}(s_3) + W_4\mathbf{b}(s_4) \qquad (3.26)$$

where $s_1 \neq s_2 \neq s_3 \neq s_4$ and W_1, W_2, W_3 and W_4 are matrices, it can be shown that

(i) <u>when $\mathbf{b}(s) = [1,1,1,\ldots,1]^T$</u>

$$W_1 + W_2 + W_3 + W_4 = M_1 \qquad (3.27)$$

where

$$M_1 = (\lambda A)^{-1}(I - exp(-\lambda l A)), \qquad (3.28)$$

(ii) when $\mathbf{b}(s) = [s, s, s, \ldots, s]^T$

$$s_1 W_1 + s_2 W_2 + s_3 W_3 + s_4 W_4 = M_2 \tag{3. 29}$$

where

$$M_2 = (\lambda A)^{-1} \Big\{ (t+l)I - t\,exp(-\lambda l A) - (\lambda A)^{-1}(I - exp(-\lambda l A)) \Big\}, \tag{3. 30}$$

(iii) when $\mathbf{b}(s) = [s^2, s^2, \ldots, s^2]^T$

$$s_1^2 W_1 + s_2^2 W_2 + s_3^2 W_3 + s_4^2 W_4 = M_3 \tag{3. 31}$$

where

$$\begin{aligned} M_3 &= (\lambda A)^{-1} \Big\{ (t+l)^2 I - t^2 exp(-\lambda l A) - 2(\lambda A)^{-1} \{ (t+l)I - t\,exp(-\lambda l A)) \\ &- (\lambda A)^{-1}(I - exp(-\lambda l A)) \} \Big\}, \end{aligned} \tag{3. 32}$$

and

(iv) when $\mathbf{b}(s) = [s^3, s^3, \ldots, s^3]^T$

$$s_1^3 W_1 + s_2^3 W_2 + s_3^3 W_3 + s_4^3 W_4 = M_4 \tag{3. 33}$$

where

$$\begin{aligned} M_4 &= (\lambda A)^{-1} \Big\{ (t+l)^3 I - t^3 exp(-\lambda l A) \\ &- 3(\lambda A)^{-1} \Big\{ (t+l)^2 I - t^2 exp(-\lambda l A) \\ &- 2(\lambda A)^{-1} \{ (t+l)I - t\,exp(lA) \\ &- (\lambda A)^{-1}(I - exp(-\lambda l A)) \} \Big\} \Big\}. \end{aligned} \tag{3. 34}$$

Solving (3.27), (3.29), (3.31) and (3.33) simultaneously gives

$$\begin{aligned} W_1 &= \left[\frac{(s_3 - s_2)(s_4 - s_2)(s_4 - s_3)}{(s_2 - s_1)(s_3 - s_1)(s_4 - s_1)(s_3 - s_2)(s_4 - s_2)(s_4 - s_3)} \right] \\ &\times \; [s_2 s_3 s_4 M_1 - (s_2 s_3 + s_2 s_4 + s_3 s_4) M_2 + (s_2 + s_3 + s_4) M_3 - M_4], \end{aligned} \tag{3. 35}$$

$$W_2 = \left[\frac{(s_3 - s_1)(s_4 - s_1)(s_4 - s_3)}{(s_2 - s_1)(s_3 - s_1)(s_4 - s_1)(s_3 - s_2)(s_4 - s_2)(s_4 - s_3)}\right] \times [s_1 s_3 s_4 M_1 - (s_1 s_3 + s_1 s_4 + s_3 s_4) M_2 + (s_1 + s_3 + s_4) M_3 - M_4], \tag{3.36}$$

$$W_3 = \left[\frac{(s_2 - s_1)(s_4 - s_1)(s_4 - s_2)}{(s_2 - s_1)(s_3 - s_1)(s_4 - s_1)(s_3 - s_2)(s_4 - s_2)(s_4 - s_3)}\right] \times [s_1 s_2 s_4 M_1 - (s_1 s_2 + s_1 s_4 + s_2 s_4) M_2 + (s_1 + s_2 + s_4) M_3 - M_4], \tag{3.37}$$

$$W_4 = \left[\frac{(s_2 - s_1)(s_3 - s_1)(s_3 - s_2)}{(s_2 - s_1)(s_3 - s_1)(s_4 - s_1)(s_3 - s_2)(s_4 - s_2)(s_4 - s_3)}\right] \times [s_1 s_2 s_3 M_1 - (s_1 s_2 + s_2 s_3 + s_1 s_3) M_2 + (s_1 + s_2 + s_3) M_3 - M_4], \tag{3.38}$$

or

$$W_1 = \left[\frac{1}{(s_2 - s_1)(s_3 - s_1)(s_4 - s_1)}\right] \times [s_2 s_3 s_4 M_1 - (s_2 s_3 + s_2 s_4 + s_3 s_4) M_2 + (s_2 + s_3 + s_4) M_3 - M_4], \tag{3.39}$$

$$W_2 = \left[\frac{1}{(s_2 - s_1)(s_3 - s_2)(s_4 - s_2)}\right] \times [s_1 s_3 s_4 M_1 - (s_1 s_3 + s_1 s_4 + s_3 s_4) M_2 + (s_1 + s_3 + s_4) M_3 - M_4], \tag{3.40}$$

$$W_3 = \left[\frac{1}{(s_3 - s_1)(s_3 - s_2)(s_4 - s_3)}\right] \times [s_1 s_2 s_4 M_1 - (s_1 s_2 + s_1 s_4 + s_2 s_4) M_2 + (s_1 + s_2 + s_4) M_3 - M_4], \tag{3.41}$$

$$W_4 = \left[\frac{1}{(s_4 - s_1)(s_4 - s_2)(s_4 - s_3)}\right] \times [s_1 s_2 s_3 M_1 - (s_1 s_2 + s_2 s_3 + s_1 s_3) M_2 + (s_1 + s_2 + s_3) M_3 - M_4]. \tag{3.42}$$

Taking $s_1 = t$, $s_2 = t + \frac{l}{2}$, $s_3 = t + \frac{2}{3}l$ and $s_4 = t + l$ gives

$$\begin{aligned} W_1 &= \frac{9}{2l^3}\left\{(t^3 + 2lt^2 + \frac{11}{9}l^2t + \frac{2}{9}l^3)M_1 - (3t^2 + 4lt + \frac{11}{9}l^2)M_2\right. \\ &+ \left.(3t + 2l)M_3 - M_4\right\}, \end{aligned} \tag{3.43}$$

$$\begin{aligned} W_2 &= -\frac{27}{2l^3}\left\{(t^3 + \frac{5}{3}lt^2 + \frac{2}{3}l^2t)M_1 - (3t^2 + \frac{10}{3}lt + \frac{2}{3}l^2)M_2\right. \\ &+ \left.(3t + \frac{5}{3}l)M_3 - M_4\right\}, \end{aligned} \tag{3.44}$$

$$\begin{aligned} W_3 &= \frac{27}{2l^3}\left\{(t^3 + \frac{4}{3}lt^2 + \frac{1}{3}l^2t)M_1 - (3t^2 + \frac{8}{3}lt + \frac{1}{3}l^2)M_2\right. \\ &+ \left.(3t + \frac{4}{3}l)M_3 - M_4\right\}, \end{aligned} \tag{3.45}$$

$$\begin{aligned} W_4 &= -\frac{9}{2l^3}\left\{(t^3 + lt^2 + \frac{2}{9}l^2t)M_1 - (3t^2 + 2lt + \frac{2}{9}l^2)M_2\right. \\ &+ \left.(3t + l)M_3 - M_4\right\}. \end{aligned} \tag{3.46}$$

Using (3.28), (3.30), (3.32) and (3.34) in (3.43)— (3.46) simultaneously gives

$$\begin{aligned} W_1 &= \frac{9}{2l^3}\left[(t^3 + 2lt^2 + \frac{11}{9}l^2t + \frac{2}{9}l^3)(\lambda A)^{-1}(I - exp(-\lambda lA))\right. \\ &- (3t^2 + 4lt + \frac{11}{9}l^2)(\lambda A)^{-1}\{(t + l)I - t\,exp(-\lambda lA) \\ &\quad - (\lambda A)^{-1}(I - exp(-\lambda lA))\} \\ &+ (3t + 2l)(\lambda A)^{-1}\left\{(t + l)^2 I - t^2 exp(-\lambda lA)\right. \\ &\quad -2(\lambda A)^{-1}\{(t + l)I - t\,exp(-\lambda lA)) \\ &\quad \left.- (\lambda A)^{-1}(I - exp(-\lambda lA))\}\right\} \\ &- (\lambda A)^{-1}\left\{(t + l)^3 I - t^3 exp(-\lambda lA)\right. \\ &\quad -3(\lambda A)^{-1}\left\{(t + l)^2 I - t^2 exp(-\lambda lA)\right. \\ &\quad -2(\lambda A)^{-1}\{(t + l)I - t\,exp(-\lambda lA) \\ &\quad \left.\left.\left.- (\lambda A)^{-1}(I - exp(-\lambda lA))\}\right\}\right\}\right], \end{aligned} \tag{3.47}$$

$$\begin{aligned} W_2 &= -\frac{27}{2l^3}\left[(t^3 + \frac{5}{3}lt^2 + \frac{2}{3}l^2t)(\lambda A)^{-1}(I - exp(-\lambda lA))\right. \\ &- (3t^2 + \frac{10}{3}lt + \frac{2}{3}l^2)(\lambda A)^{-1}\{(t + l)I - t\,exp(-\lambda lA) \end{aligned}$$

$$
\begin{aligned}
& - (\lambda A)^{-1}(I - exp(-\lambda l A))\Big\} \\
+ \quad & (3t + \frac{5}{3}l)(\lambda A)^{-1}\Big\{(t+l)^2 I - t^2 exp(-\lambda l A) \\
& -2(\lambda A)^{-1}\{(t+l)I - t\,exp(-\lambda l A)) \\
& - (\lambda A)^{-1}(I - exp(-\lambda l A))\Big\}\Big\} \\
- \quad & (\lambda A)^{-1}\Big\{(t+l)^3 I - t^3 exp(-\lambda l A) \\
& -3(\lambda A)^{-1}\Big\{(t+l)^2 I - t^2 exp(-\lambda l A) \\
& -2(\lambda A)^{-1}\{(t+l)I - t\,exp(-\lambda l A) \\
& - (\lambda A)^{-1}(I - exp(-\lambda l A))\Big\}\Big\}\Big\}\Big], \qquad (3.48)
\end{aligned}
$$

$$
\begin{aligned}
W_3 = \quad & \frac{27}{2l^3}\Big[(t^3 + \frac{4}{3}lt^2 + \frac{1}{3}l^2 t)(\lambda A)^{-1}(I - exp(-\lambda l A)) \\
- \quad & (3t^2 + \frac{8}{3}lt + \frac{1}{3}l^2)(\lambda A)^{-1}\{(t+l)I - t\,exp(-\lambda l A) \\
& - (\lambda A)^{-1}(I - exp(-\lambda l A))\Big\} \\
+ \quad & (3t + \frac{4}{3}l)(\lambda A)^{-1}\Big\{(t+l)^2 I - t^2 exp(-\lambda l A) \\
& -2(\lambda A)^{-1}\{(t+l)I - t\,exp(-\lambda l A)) \\
& - (\lambda A)^{-1}(I - exp(-\lambda l A))\Big\}\Big\} \\
- \quad & (\lambda A)^{-1}\Big\{(t+l)^3 I - t^3 exp(-\lambda l A) \\
& -3(\lambda A)^{-1}\Big\{(t+l)^2 I - t^2 exp(-\lambda l A) \\
& -2(\lambda A)^{-1}\{(t+l)I - t\,exp(-\lambda l A) \\
& - (\lambda A)^{-1}(I - exp(-\lambda l A))\Big\}\Big\}\Big\}\Big], \qquad (3.49)
\end{aligned}
$$

$$
\begin{aligned}
W_4 = - \quad & \frac{9}{2l^3}\Big[(t^3 + lt^2 + \frac{2}{9}l^2 t)(\lambda A)^{-1}(I - exp(-\lambda l A)) \\
- \quad & (3t^2 + 2lt + \frac{2}{9}l^2)(\lambda A)^{-1}\{(t+l)I - t\,exp(-\lambda l A) \\
& - (\lambda A)^{-1}(I - exp(-\lambda l A))\Big\} \\
+ \quad & (3t + l)(\lambda A)^{-1}\Big\{(t+l)^2 I - t^2 exp(-\lambda l A) \\
& -2(\lambda A)^{-1}\{(t+l)I - t\,exp(-\lambda l A))
\end{aligned}
$$

$$
\begin{aligned}
& - (\lambda A)^{-1}(I - exp(-\lambda l A))\Big\}\Big\} \\
- \quad & (\lambda A)^{-1}\Big\{(t+l)^3 I - t^3 exp(-\lambda l A) \\
& -3(\lambda A)^{-1}\Big\{(t+l)^2 I - t^2 exp(-\lambda l A) \\
& -2(\lambda A)^{-1}\{(t+l)I - t\, exp(-\lambda l A) \\
& - (\lambda A)^{-1}(I - exp(-\lambda l A))\Big\}\Big\}\Big\}\Big], \qquad (3.50)
\end{aligned}
$$

or

$$
\begin{aligned}
W_1 \;=\; & \frac{9}{2l^3}[(\lambda A)^{-1}]^4\Big[(t^3 + 2lt^2 + \frac{11}{9}l^2 t + \frac{2}{9}l^3)(\lambda A)^3(I - exp(-\lambda l A)) \\
- \;& (3t^2 + 4lt + \frac{11}{9}l^2)(\lambda A)^3((t+l)I - t\, exp(-\lambda l A)) \\
+ \;& (3t^2 + 4lt + \frac{11}{9}l^2)(\lambda A)^2(I - exp(-\lambda l A)) \\
+ \;& (3t + 2l)(\lambda A)^3((t+l)^2 I - t^2 exp(-\lambda l A)) \\
- \;& 2(3t + 2l)(\lambda A)^2((t+l)I - t\, exp(-\lambda l A)) \\
+ \;& 2(3t + 2l)(\lambda A)(I - exp(-\lambda l A)) \\
- \;& (\lambda A)^3((t+l)^3 I - t^3 exp(-\lambda l A)) \\
+ \;& 3(\lambda A)^2((t+l)^2 I - t^2 exp(-\lambda l A)) \\
- \;& 6(\lambda A)((t+l)I - t\, exp(-\lambda l A)) \\
+ \;& 6(I - exp(-\lambda l A))\Big], \qquad (3.51)
\end{aligned}
$$

$$
\begin{aligned}
W_2 \;=\; & -\frac{27}{2l^3}[(\lambda A)^{-1}]^4\Big[(t^3 + \frac{5}{3}lt^2 + \frac{2}{3}l^2 t)(\lambda A)^3(I - exp(-\lambda l A)) \\
- \;& (3t^2 + \frac{10}{3}lt + \frac{2}{3}l^2)(\lambda A)^3((t+l)I - t\, exp(-\lambda l A)) \\
+ \;& (3t^2 + \frac{10}{3}lt + \frac{2}{3}l^2)(\lambda A)^2(I - exp(-\lambda l A)) \\
+ \;& (3t + \frac{5}{3}l)(\lambda A)^3((t+l)^2 I - t^2 exp(-\lambda l A)) \\
- \;& 2(3t + \frac{5}{3}l)(\lambda A)^2((t+l)I - t\, exp(-\lambda l A)) \\
+ \;& 2(3t + \frac{5}{3}l)(\lambda A)(I - exp(-\lambda l A))
\end{aligned}
$$

$$
\begin{aligned}
&- (\lambda A)^3((t+l)^3 I - t^3\, exp(-\lambda l A)) \\
&+ 3(\lambda A)^2((t+l)^2 I - t^2\, exp(-\lambda l A)) \\
&- 6(\lambda A)((t+l) I - t\, exp(-\lambda l A)) \\
&+ 6(I - exp(-\lambda l A))\Big], \qquad (3.52)
\end{aligned}
$$

$$
\begin{aligned}
W_3 &= \frac{27}{2l^3}[(\lambda A)^{-1}]^4 \Big[(t^3 + \frac{4}{3}lt^2 + \frac{1}{3}l^2 t)(\lambda A)^3 (I - exp(-\lambda l A)) \\
&- (3t^2 + \frac{8}{3}lt + \frac{1}{3}l^2)(\lambda A)^3((t+l)I - t\, exp(-\lambda l A)) \\
&+ (3t^2 + \frac{8}{3}lt + \frac{1}{3}l^2)(\lambda A)^2(I - exp(-\lambda l A)) \\
&+ (3t + \frac{4}{3}l)(\lambda A)^3((t+l)^2 I - t^2\, exp(-\lambda l A)) \\
&- 2(3t + \frac{4}{3}l)(\lambda A)^2((t+l)I - t\, exp(-\lambda l A)) \\
&+ 2(3t + \frac{4}{3}l)(\lambda A)(I - exp(-\lambda l A)) \\
&- (\lambda A)^3((t+l)^3 I - t^3\, exp(-\lambda l A)) \\
&+ 3(\lambda A)^2((t+l)^2 I - t^2\, exp(-\lambda l A)) \\
&- 6(\lambda A)((t+l) I - t\, exp(-\lambda l A)) \\
&+ 6(I - exp(-\lambda l A))\Big], \qquad (3.53)
\end{aligned}
$$

$$
\begin{aligned}
W_4 &= -\frac{9}{2l^3}[(\lambda A)^{-1}]^4 \Big[(t^3 + lt^2 + \frac{2}{9}l^2 t)(\lambda A)^3 (I - exp(-\lambda l A)) \\
&- (3t^2 + 2lt + \frac{2}{9}l^2)(\lambda A)^3((t+l)I - t\, exp(-\lambda l A)) \\
&+ (3t^2 + 2lt + \frac{2}{9}l^2)(\lambda A)^2(I - exp(-\lambda l A)) \\
&+ (3t + l)(\lambda A)^3((t+l)^2 I - t^2\, exp(-\lambda l A)) \\
&- 2(3t + l)(\lambda A)^2((t+l)I - t\, exp(-\lambda l A)) \\
&+ 2(3t + l)(\lambda A)(I - exp(-\lambda l A)) \\
&- (\lambda A)^3((t+l)^3 I - t^3\, exp(-\lambda l A)) \\
&+ 3(\lambda A)^2((t+l)^2 I - t^2\, exp(-\lambda l A))
\end{aligned}
$$

$$- \quad 6(\lambda A)((t+l)I - t\,exp(-\lambda l A))$$

$$+ \quad 6(I - exp(-\lambda l A))]. \qquad (3.54)$$

Simplification gives

$$\begin{aligned}
W_1 &= \frac{9}{2l^3}((\lambda A)^{-1})^4 \left[\left\{t^3 + 2lt^2 + \frac{11}{9}l^2 t + \frac{2}{9}l^3 - (t+l)(3t^2 + 4lt + \frac{11}{9}l^2)\right.\right. \\
&\quad \left. + (3t+2l)(t+l)^2 - (t+l)^3\right\}(\lambda A)^3 \\
&+ \left\{3t^2 + 4lt + \frac{11}{9}l^2 - 2(3t+2l)(t+l) + 3(t+l)^2\right\}(\lambda A)^2 \\
&+ \{2(3t+2l) - 6(t+l)\}(\lambda A) + 6I \\
&+ \left\{\left\{-(t^3 + 2lt^2 + \frac{11}{9}l^2 t + \frac{2}{9}l^3) + t(3t^2 + 4lt + \frac{11}{9}l^2)\right.\right. \\
&\quad \left. - (3t+2l)t^2 + t^3\right\}(\lambda A)^3 \\
&+ \left\{-(3t^2 + 4lt + \frac{11}{9}l^2) + 2t(3t+2l) - 3t^2\right\}(\lambda A)^2 \\
&+ \{-2(3t+2l) + 6t)\}(\lambda A) - 6I\}\, exp(-\lambda A)], \qquad (3.55)
\end{aligned}$$

$$\begin{aligned}
W_2 &= -\frac{27}{2l^3}((\lambda A)^{-1})^4 \left[\left\{t^3 + \frac{5}{3}lt^2 + \frac{2}{3}l^2 t - (t+l)(3t^2 + \frac{10}{3}lt + \frac{2}{3}l^2)\right.\right. \\
&\quad \left. + (3t + \frac{5}{3}l)(t+l)^2 - (t+l)^3\right\}(\lambda A)^3 \\
&+ \left\{3t^2 + \frac{10}{3}lt + \frac{2}{3}l^2 - 2(3t + \frac{5}{3}l)(t+l) + 3(t+l)^2\right\}(\lambda A)^2 \\
&+ \left\{2(3t + \frac{5}{3}l) - 6(t+l)\right\}(\lambda A) + 6I \\
&+ \left\{\left\{-(t^3 + \frac{5}{3}lt^2 + \frac{2}{3}l^2 t) + t(3t^2 + \frac{10}{3}lt + \frac{2}{3}l^2)\right.\right. \\
&\quad \left. - (3t + \frac{5}{3}l)t^2 + t^3\right\}(\lambda A)^3 \\
&+ \left\{-(3t^2 + \frac{10}{3}lt + \frac{2}{3}l^2) + 2t(3t + \frac{5}{3}l) - 3t^2\right\}(\lambda A)^2 \\
&+ \left.\left\{-2(3t + \frac{5}{3}l) + 6t)\right\}(\lambda A) - 6I\right\} exp(-\lambda A)\Big], \qquad (3.56)
\end{aligned}$$

$$\begin{aligned}
W_3 &= \frac{27}{2l^3}((\lambda A)^{-1})^4 \left[\left\{t^3 + \frac{4}{3}lt^2 + \frac{1}{3}l^2 t - (t+l)(3t^2 + \frac{8}{3}lt + \frac{1}{3}l^2)\right.\right. \\
&\quad \left. + (3t + \frac{4}{3}l)(t+l)^2 - (t+l)^3\right\}(\lambda A)^3
\end{aligned}$$

$$
\begin{aligned}
&+ \left\{3t^2 + \frac{8}{3}lt + \frac{1}{3}l^2 - 2(3t + \frac{4}{3}l)(t+l) + 3(t+l)^2\right\}(\lambda A)^2 \\
&+ \left\{2(3t + \frac{4}{3}l) - 6(t+l)\right\}(\lambda A) + 6I \\
&+ \left\{\left\{-(t^3 + \frac{4}{3}lt^2 + \frac{1}{3}l^2 t) + t(3t^2 + \frac{8}{3}lt + \frac{1}{3}l^2)\right.\right. \\
&\quad \left. - (3t + \frac{4}{3}l)t^2 + t^3\right\}(\lambda A)^3 \\
&+ \left\{-(3t^2 + \frac{8}{3}lt + \frac{1}{3}l^2) + 2t(3t + \frac{4}{3}l) - 3t^2\right\}(\lambda A)^2 \\
&+ \left.\left\{-2(3t + \frac{4}{3}l) + 6t)\right\}(\lambda A) - 6I\right\} exp(-\lambda A)\Big], \qquad (3.57)
\end{aligned}
$$

$$
\begin{aligned}
W_4 &= -\frac{9}{2l^3}((\lambda A)^{-1})^4 \Big[\Big\{t^3 + lt^2 + \frac{2}{9}l^2 t - (t+l)(3t^2 + 2lt + \frac{2}{9}l^2) \\
&\quad + (3t+l)(t+l)^2 - (t+l)^3\Big\}(\lambda A)^3 \\
&+ \left\{3t^2 + 2lt + \frac{2}{9}l^2 - 2(3t+l)(t+l) + 3(t+l)^2\right\}(\lambda A)^2 \\
&+ \{2(3t+l) - 6(t+l)\}(\lambda A) + 6I \\
&+ \Big\{\Big\{-(t^3 + lt^2 + \frac{2}{9}l^2 t) + t(3t^2 + 2lt + \frac{2}{9}l^2) \\
&\quad - (3t+l)t^2 + t^3\Big\}(\lambda A)^3 \\
&+ \left\{-(3t^2 + 2lt + \frac{2}{9}l^2) + 2t(3t+l) - 3t^2\right\}(\lambda A)^2 \\
&+ \{-2(3t+l) + 6t)\}(\lambda A) - 6I\} exp(-\lambda A)]. \qquad (3.58)
\end{aligned}
$$

Then it is easy to show that

$$
\begin{aligned}
W_1 &= \frac{9}{2l^3}[(\lambda A)^{-1}]^4 \Big\{6I - 2\lambda lA + \frac{2}{9}(\lambda lA)^2 \\
&- \left(6I + 4\,\lambda lA + \frac{11}{9}(\lambda lA)^2 + \frac{2}{9}(\lambda lA)^3\right) exp(-\lambda lA)\Big\}, \qquad (3.59) \\
W_2 &= -\frac{27}{2l^3}[(\lambda A)^{-1}]^4 \Big\{6I - \frac{8}{3}\lambda lA + \frac{1}{3}(\lambda lA)^2 \\
&- \left(6I + \frac{10}{3}\lambda lA + \frac{2}{3}(\lambda lA)^2\right) exp(-\lambda lA)\Big\}, \qquad (3.60) \\
W_3 &= \frac{27}{2l^3}[(\lambda A)^{-1}]^4 \Big\{6I - \frac{10}{3}\lambda lA + \frac{2}{3}(\lambda lA)^2 \\
&- \left(6I + \frac{8}{3}\lambda lA + \frac{1}{3}(\lambda lA)^2\right) exp(-\lambda lA)\Big\}, \qquad (3.61)
\end{aligned}
$$

$$
\begin{aligned}
W_4 &= -\frac{9}{2l^3}[(\lambda A)^{-1}]^4\left\{6I - 4\lambda lA + \frac{11}{9}(\lambda lA)^2 - \frac{2}{9}(\lambda lA)^3\right. \\
&- \left.\left(6I + 2\lambda lA + \frac{2}{9}(\lambda lA)^2\right)exp(-\lambda lA)\right\}. \qquad (3.62)
\end{aligned}
$$

Using (3.23) in (3.59)—(3.62) gives

$$
\begin{aligned}
W_1 &= \frac{l}{24}\{(3I - (-19 + 78a_1 - 216a_2 + 324a_3)\lambda lA \\
&+(3 - 8a_1 + 12a_2)(\lambda lA)^2\} D^{-1}, \qquad (3.63) \\
W_2 &= \frac{3}{16}l\{(2I + (-16 + 56a_1 - 144a_2 + 216a_3)\lambda lA \\
&+(1 - 4a_1 + 12a_2 - 24a_3)(\lambda lA)^2\} D^{-1}, \qquad (3.64) \\
W_3 &= \frac{3}{8}l\{(I + (7 - 26a_1 + 72a_2 - 108a_3)\lambda lA \\
&-(1 - 4a_1 + 12a_2 - 24a_3)(\lambda lA)^2\} D^{-1}, \qquad (3.65) \\
W_4 &= \frac{l}{48}l\{(6I - (44 - 168a_1 + 432a_2 - 648a_3)\lambda lA \\
&+(11 - 44a_1 + 132a_2 - 216a_3)(\lambda lA)^2 \\
&- (2 - 8a_1 + 24a_2 - 48a_3)(\lambda lA)^3\} D^{-1}. \qquad (3.66)
\end{aligned}
$$

Hence (3.22) can be written as

$$
\mathrm{U}(t+l) = exp(-\lambda lA)\mathrm{U}(t) + W_1\mathrm{b}(t) + W_2\mathrm{b}(t+\frac{l}{3}) + W_3\mathrm{b}(t+\frac{2}{3}l) + W_4\mathrm{b}(t+l). \qquad (3.67)
$$

3.2 Algorithm

Assuming that r_1, r_2, r_3 and r_4 are the real zeros of

$$
q(\theta) = 1 + a_1\theta + a_2\theta^2 + a_3\theta^3 + (-\frac{1}{24} + \frac{a_1}{6} - \frac{a_2}{2} + a_3)\theta^4 \qquad (3.68)
$$

then D given by (3.24) can be factorized as

$$
D = (I - \frac{\lambda l}{r_1}A)(I - \frac{\lambda l}{r_2}A)(I - \frac{\lambda l}{r_3}A)(I - \frac{\lambda l}{r_4}A), \qquad (3.69)
$$

and then (3.67) can be written in partial-fraction form as

$$\begin{aligned} \mathbf{U}(t+l) &= \Big\{ A_1(I - \frac{\lambda l}{r_1}A)^{-1} + A_2(I - \frac{\lambda l}{r_2}A)^{-1} \\ &\quad + A_3(I - \frac{\lambda l}{r_3}A)^{-1} + A_4(I - \frac{\lambda l}{r_4}A)^{-1} \Big\} \mathbf{U}(t) \\ &+ \frac{l}{24} \Big\{ B_1(I - \frac{\lambda l}{r_1}A)^{-1} + B_2(I - \frac{\lambda l}{r_2}A)^{-1} \\ &\quad + B_3(I - \frac{\lambda l}{r_3}A)^{-1} + B_4(I - \frac{\lambda l}{r_4}A)^{-1} \Big\} \mathbf{b}(t) \\ &+ \frac{3}{16} l \Big\{ C_1(I - \frac{\lambda l}{r_1}A)^{-1} + C_2(I - \frac{\lambda l}{r_2}A)^{-1} \\ &\quad + C_3(I - \frac{\lambda l}{r_3}A)^{-1} + C_4(I - \frac{\lambda l}{r_4}A)^{-1} \Big\} \mathbf{b}(t + \frac{l}{3}) \\ &+ \frac{3}{8} l \Big\{ D_1(I - \frac{\lambda l}{r_1}A)^{-1} + D_2(I - \frac{\lambda l}{r_2}A)^{-1} \\ &\quad + D_3(I - \frac{\lambda l}{r_3}A)^{-1} + D_4(I - \frac{\lambda l}{r_4}A)^{-1} \Big\} \mathbf{b}(t + \frac{2}{3} l) \\ &+ \frac{l}{48} \Big\{ E_1(I - \frac{\lambda l}{r_1}A)^{-1} + E_2(I - \frac{\lambda l}{r_2}A)^{-1} \\ &\quad + E_3(I - \frac{\lambda l}{r_3}A)^{-1} + E_4(I - \frac{\lambda l}{r_4}A)^{-1} \Big\} \mathbf{b}(t + l) \quad (3.70) \end{aligned}$$

in which, for $i = 1, 2, 3, 4$,

$$\begin{aligned} A_i &= \frac{1 - p_1 r_i + p_2 r_i^2 - p_3 r_i^3}{\prod_{j=1, j \neq i}^{4} (1 - \frac{r_i}{r_j})}, \\ B_i &= \frac{3 - p_4 r_i + p_5 r_i^2}{\prod_{j=1, j \neq i}^{4} (1 - \frac{r_i}{r_j})}, \\ C_i &= \frac{2 - p_6 r_i + p_7 r_i^2}{\prod_{j=1, j \neq i}^{4} (1 - \frac{r_i}{r_j})}, \\ D_i &= \frac{1 - p_8 r_i - p_9 r_i^2}{\prod_{j=1, j \neq i}^{4} (1 - \frac{r_i}{r_j})}, \end{aligned}$$

$$E_i = \frac{6 - p_{10} r_i + p_{11} r_i^2 - p_{12} r_i^3}{\prod_{\substack{j=1 \\ j \neq i}}^{4} (1 - \frac{r_i}{r_j})}$$

where

$$\begin{aligned}
p_1 &= 1 - a_1 \\
p_2 &= \frac{1}{2} - a_1 + a_2 \\
p_3 &= \frac{1}{6} - \frac{a_1}{2} + a_2 - a_3 \\
p_4 &= -19 + 78a_1 - 216a_2 + 324a_3 \\
p_5 &= 3 - 8a_1 + 12a_2 \\
p_6 &= 16 - 56a_1 + 144a_2 - 216a_3 \\
p_7 &= 1 - 4a_1 + 12a_2 - 24a_3 \\
p_8 &= -7 + 26a_1 - 72a_2 + 108a_3 \\
p_9 &= 1 - 4a_1 + 12a_2 - 24a_3 \\
p_{10} &= 44 - 168a_1 + 432a_2 - 648a_3 \\
p_{11} &= 11 - 44a_1 + 132a_2 - 216a_3 \\
p_{12} &= 2 - 8a_1 + 24a_2 - 48a_3.
\end{aligned}$$

Then

$$\begin{aligned}
\mathbf{U}(t+l) &= (I - \frac{1}{r_1}\lambda l A)^{-1} \Big[A_1 \mathbf{U}(t) + \frac{l}{24}(B_1 \mathbf{b}(t) + \frac{3}{16} l C_1 \mathbf{b}(t + \frac{l}{3}) \\
&\quad + \frac{3}{8} l D_1 \mathbf{b}(t + \frac{2}{3} l) + \frac{l}{48} E_1 \mathbf{b}(t+l)) \Big] \\
&+ (I - \frac{1}{r_2}\lambda l A)^{-1} \Big[A_2 \mathbf{U}(t) + \frac{l}{24}(B_2 \mathbf{b}(t) + \frac{3}{16} l C_2 \mathbf{b}(t + \frac{l}{3}) \\
&\quad + \frac{3}{8} l D_2 \mathbf{b}(t + \frac{2}{3} l) + \frac{l}{48} E_2 \mathbf{b}(t+l)) \Big] \\
&+ (I - \frac{1}{r_3}\lambda l A)^{-1} \Big[A_3 \mathbf{U}(t) + \frac{l}{24}(B_3 \mathbf{b}(t) + \frac{3}{16} l C_3 \mathbf{b}(t + \frac{l}{3})
\end{aligned}$$

$$+ \frac{3}{8}lD_3\mathbf{b}(t+\frac{2}{3}l) + \frac{l}{48}E_3\mathbf{b}(t+l))\Big]$$

$$+ \quad (I - \frac{1}{r_4}\lambda lA)^{-1}\Big[A_4\mathbf{U}(t) + \frac{l}{24}(B_4\mathbf{b}(t) + \frac{3}{16}lC_4\mathbf{b}(t+\frac{l}{3})$$

$$+ \frac{3}{8}lD_4\mathbf{b}(t+\frac{2}{3}l) + \frac{l}{48}E_4\mathbf{b}(t+l))\Big] \qquad (3.71)$$

which gives

$$\begin{aligned} \mathbf{U}(t+l) &= (I - \frac{1}{r_1}\lambda lA)^{-1}\mathbf{z}_1 + (I - \frac{1}{r_i}\lambda lA)^{-1}\mathbf{z}_2 \\ &+ (I - \frac{1}{r_3}\lambda lA)^{-1}\mathbf{z}_3 + (I - \frac{1}{r_4}\lambda lA)^{-1}\mathbf{z}_4, \end{aligned} \qquad (3.72)$$

where

$$\begin{aligned} \mathbf{z}_i &= A_i\mathbf{U}(t) + \frac{l}{24}(B_i\mathbf{b}(t) + \frac{3}{16}lC_i\mathbf{b}(t+\frac{l}{3}) \\ &+ \frac{3}{8}lD_i\mathbf{b}(t+\frac{2}{3}l) + \frac{l}{48}E_i\mathbf{b}(t+l)) \quad i = 1,2,3,4. \end{aligned}$$

Let

$$(I - \frac{1}{r_i}\lambda lA)^{-1}\mathbf{z}_i = \mathbf{y}_i, \quad i = 1,2,3,4$$

then

$$(I - \frac{1}{r_i}\lambda lA)\mathbf{y}_i = \mathbf{z}_i, \quad i = 1,2,3,4 \qquad (3.73)$$

and

$$\mathbf{U}(t+l) = \mathbf{y}_1 + \mathbf{y}_2 + \mathbf{y}_3 + \mathbf{y}_4 \qquad (3.74)$$

in which $\mathbf{y}_1$, $\mathbf{y}_2$, $\mathbf{y}_3$ and $\mathbf{y}_4$ are the solutions of the systems

$$(I - \frac{1}{r_i}\lambda lA)\mathbf{y}_i = \mathbf{z}_i, \quad i = 1,2,3,4 \qquad (3.75)$$

respectively. This algorithm is presented in tabular form in Table 3.1.

3.3 Numerical Examples

In this section a representative of many other methods based on (3.23) will be used. So taking

$$a_1 = \frac{64}{25}$$
$$a_2 = \frac{7}{3}$$

and

$$a_3 = \frac{547}{600}$$

Taj and Twizell [39], which give a small local trunction error, it is found that

r_1=-0.937580908085238, r_2=-1.81471985800593,
r_3=-2.00000000000000, r_4=-2.26051974672921

are the real zeros of (3.24). These values produce

A_1= 0.211455566708523, A_2= -53.3503067445635,
A_3= 108.000000000009, A_4= -53.8611488221542,
B_1= -92.8251781374359, B_2= 764.030220887627,
B_3=-810.000000000074, B_4= 141.794957249882,
C_1= 68.1850562754185, C_2=-760.226330382964,
C_3=972.000000000087, C_4=-277.958725892541,
D_1= -37.3634484931730, D_2= 399.961234456715,
D_3=-486.000000000044, D_4= 124.402214036502,
E_1= 255.352513419023, E_2=-3296.46069786871,
E_3=4212.00000000038, E_4=-1164.89181555069

3.3.1 Example 1

Consider the one space variable partial differential equation

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0, \quad 0 < x < 1, \quad t > 0. \qquad (3.76)$$

subject to the boundary conditions

$$u(0,t) = -sin(2k\pi t), \quad t > 0, \tag{3. 77}$$

where k is a positive integer and the initial condition

$$u(x,0) = sin(2k\pi x), \quad 0 \leq x \leq 1. \tag{3. 78}$$

This problem has theoretical solution

$$u(x,t) = sin[2k\pi(x-t)] \tag{3. 79}$$

(see Oliger [31]). The integer k gives the number of complete waves in the interval $0 \leq x \leq 1$. Using the Algorithm 1 with the information given at the beginning of this section the problem {(3.76)-(3.78)} is solved for $h = \frac{1}{640}$ and $l = \frac{1}{80}$ so that $r = 8.0(r = \frac{l}{h})$, using $k = 2$ and 4 and compared with the results obtained by Arigu *et al.* [5] whose method requires the use of complex arithmatic. The numerical solutions for $k = 2$ and $k = 4$ at time $t = 1.0$ and t=10.0 respectively are depicted in Figure 3.1 and Figure 3.2. In these experiments the method behaves smoothly over the whole interval $0 \leq x \leq 1$ and no oscillations are observed. Maximum errors at time t=0.5, 1.0, 2.0, 4.0, 10.0, are given in Table 3.2.

3.3.2 Example 2

Consider again the one space variable partial differential equation (3.2)

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0, \quad 0 < x < 1, \quad t > 0. \tag{3. 80}$$

subject to the boundary conditions

$$u(0,t) = e^{-t}, \quad t > 0, \tag{3. 81}$$

and the initial condition

$$u(x,0) = e^x, \quad 0 \le x \le 1. \tag{3.82}$$

This problem has theoretical solution

$$u(x,t) = e^{x-t} \tag{3.83}$$

(see Arigu *et al.* [5]), which decays as time increases. Using once again the algorithm developed in Section 3.2 with the information given at the beginning of this section the problem {(3.80)–(3.82)} is solved for $h = \frac{1}{80}$ and $l = \frac{1}{120}$ and compared once again with the results obtained by Arigu *et al.* [5]. The numerical solutions at time t=1.0 and t=10.0 are depicted in Figure 3.3 and Figure 3.4 respectively. In these experiments the method behaves smoothly over the whole interval $0 \le x \le 1$ and no contrived oscillations are observed. Maximum errors at time t=0.5, 1.0, 2.0, 4.0 and 10.0 are given in Table 3.3. In addition, the experiments are performed for h, l=0.1, 0.05, 0.025, 0.0125 at time t=1.0, 10.0 and it is noted from Table 3.4 that the method is fourth-order accurate for large values of h and l because, as h and l are both successively halved, the error decreases in magnitude by a factor of 16(approximately). However, the accuracy is affected for smaller values of h and l because so many arithmetic operations cause an accumulation of round-off error.

Table 3.1: Algorithm 1

Steps	Processor 1	Processor 2	Processor 3	Processor 4
1 Input	$l, r_1, \mathbf{U}_0, A, A_1$ B_1, C_1, D_1, E_1	$l, r_2, \mathbf{U}_0, A, A_2$ B_2, C_2, D_2, E_2	$l, r_3, \mathbf{U}_0, A, A_3$ B_3, C_3, D_3, E_3	$l, r_4, \mathbf{U}_0, A, A_4$ B_4, C_4, D_4, E_4
2 Comp	$I - \frac{\lambda l}{r_1} A$	$I - \frac{\lambda l}{r_2} A$	$I - \frac{\lambda l}{r_3} A$	$I - \frac{\lambda l}{r_4} A$
3 Decom	$I - \frac{\lambda l}{r_1} A$ $= L_1 U_1$	$I - \frac{\lambda l}{r_2} A$ $= L_2 U_2$	$I - \frac{\lambda l}{r_3} A$ $= L_3 U_3$	$I - \frac{\lambda l}{r_4} A$ $= L_4 U_4$
4 Comp	$\mathbf{b}_1 = \mathbf{b}(t)$ $\mathbf{b}_2 = \mathbf{b}(t + \frac{l}{3})$ $\mathbf{b}_3 = \mathbf{b}(t + \frac{2l}{3})$ $\mathbf{b}_4 = \mathbf{b}(t + l)$	$\mathbf{b}_1 = \mathbf{b}(t)$ $\mathbf{b}_2 = \mathbf{b}(t + \frac{l}{3})$ $\mathbf{b}_3 = \mathbf{b}(t + \frac{2l}{3})$ $\mathbf{b}_4 = \mathbf{b}(t + l)$	$\mathbf{b}_1 = \mathbf{b}(t)$ $\mathbf{b}_2 = \mathbf{b}(t + \frac{l}{3})$ $\mathbf{b}_3 = \mathbf{b}(t + \frac{2l}{3})$ $\mathbf{b}_4 = \mathbf{b}(t + l)$	$\mathbf{b}_1 = \mathbf{b}(t)$ $\mathbf{b}_2 = \mathbf{b}(t + \frac{l}{3})$ $\mathbf{b}_3 = \mathbf{b}(t + \frac{2l}{3})$ $\mathbf{b}_4 = \mathbf{b}(t + l)$
5 Using	$\mathbf{w}_1(t)$ $= \frac{l}{48}\{2B_1\mathbf{b}_1$ $+9C_1\mathbf{b}_2$ $+18D_1\mathbf{b}_3$ $+E_1\mathbf{b}_4\}$	$\mathbf{w}_2(t)$ $= \frac{l}{48}\{2B_2\mathbf{b}_1$ $+9C_2\mathbf{b}_2$ $+18D_2\mathbf{b}_3$ $+E_2\mathbf{b}_4\}$	$\mathbf{w}_3(t)$ $= \frac{l}{48}\{2B_3\mathbf{b}_1$ $+9C_3\mathbf{b}_2$ $+18D_3\mathbf{b}_3$ $+E_3\mathbf{b}_4\}$	$\mathbf{w}_4(t)$ $= \frac{l}{48}\{2B_4\mathbf{b}_1$ $+9C_4 1\mathbf{b}_2$ $+18D_4\mathbf{b}_3$ $+E_4\mathbf{b}_4\}$
6 Solve	$L_1U_1\mathbf{y}_1(t)$ $= A_1\mathbf{U}(t)$ $+\mathbf{w}_1(t)$	$L_2U_2\mathbf{y}_2(t)$ $= A_2\mathbf{U}(t)$ $+\mathbf{w}_2(t)$	$L_3U_3\mathbf{y}_3(t)$ $= A_3\mathbf{U}(t)$ $+\mathbf{w}_3(t)$	$L_4U_4\mathbf{y}_4(t)$ $= A_4\mathbf{U}(t)$ $+\mathbf{w}_4(t)$
7	$\mathbf{U}(t + l) = \mathbf{y}_1(t) + \mathbf{y}_2(t) + \mathbf{y}_3(t) + \mathbf{y}_4(t)$			
8	GO TO Step 4 for next time step			

Table 3.2: Maximum errors for Example 1 at $t = 0.5, 1.0, 2.0, 4.0, 10$

t	0.5	1.0	2.0	4.0	10.0
k=2	-0.132D-3	0.241D-3	0.242D-3	0.242D-3	0.242D-3
*	0.271D-2	0.269D-1	0.261D-1	0.260D-2	—
k=4	-0.395D-2	-0.693D-2	-0.693D-2	-0.693D-2	-0.693D-2
*	—	—	—	—	0.641D-1

* Maximum absolute errors of Arigu *et al.* $O(h^2 + l^3)$ Method

Table 3.3: Maximum errors for Example 2 at $t = 0.5, 1.0, 2.0, 4.0, 10.0$

t	0.5	1.0	2.0	4.0	10.0
	0.41905D-6	-0.28270D-7	-0.57121D-8	-0.43606D-9	-0.14274D-11
*	—	—	0.511D-2	0.215D-4	0.869D-6

* Maximum absolute errors of Arigu *et al.* $O(h^2 + l^4)$ Method

Table 3.4: Maximum errors showing fourth-order accuracy for Example 2 at t=1.0 and 10.0

h, l	0.1	0.05	0.025	0.0125
t = 1.0	-0.13664D-4	-0.81996D-6	-0.46864D-7	-0.58554D-8
t = 10.0	-0.17417D-8	-0.99378D-10	-0.61453D-11	-0.99222D-12

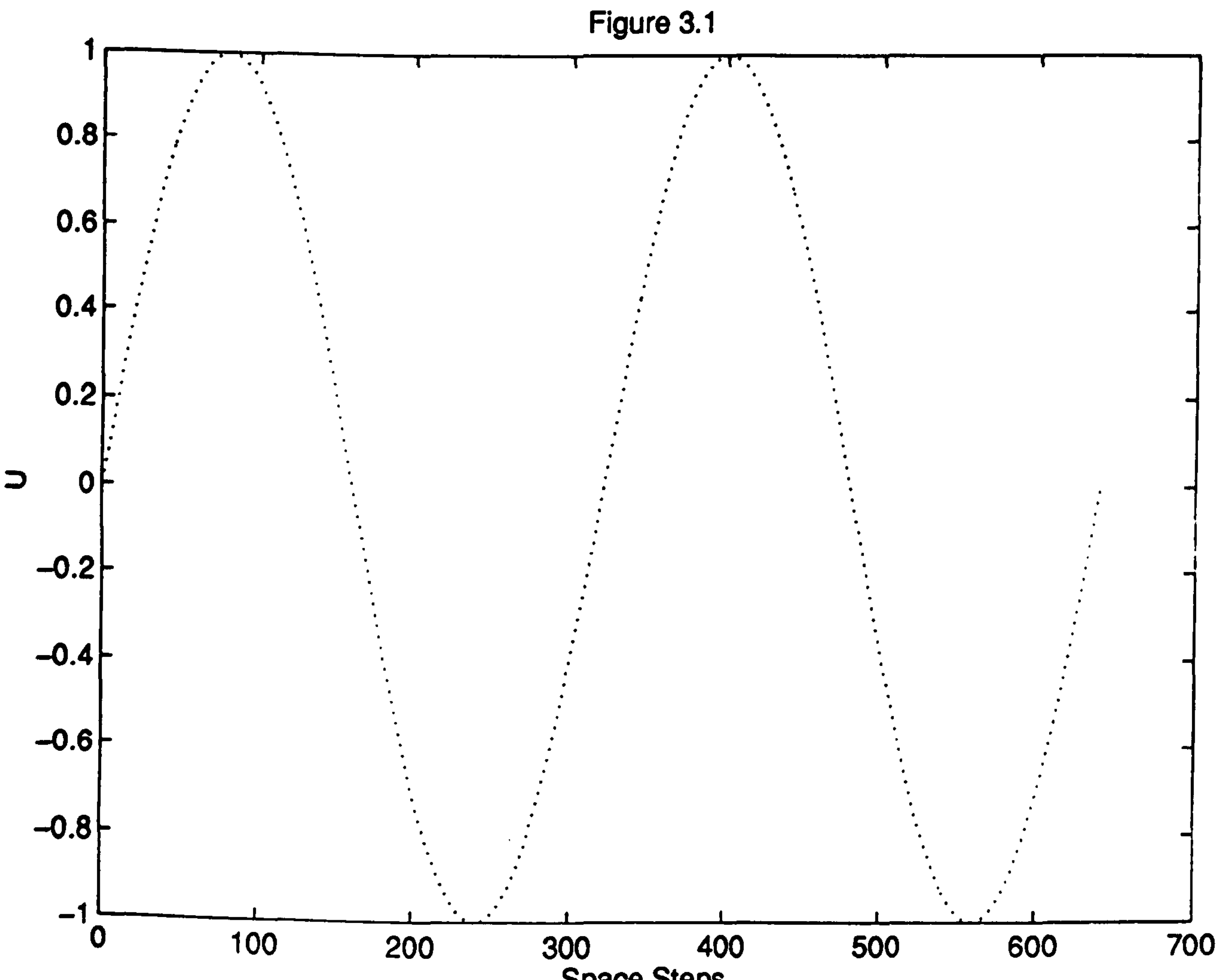

Figure 3.1: Numerical solution of example 1 for $k = 2$, $h = \frac{1}{640}$ and $l = \frac{1}{80}$ at time t=0.5

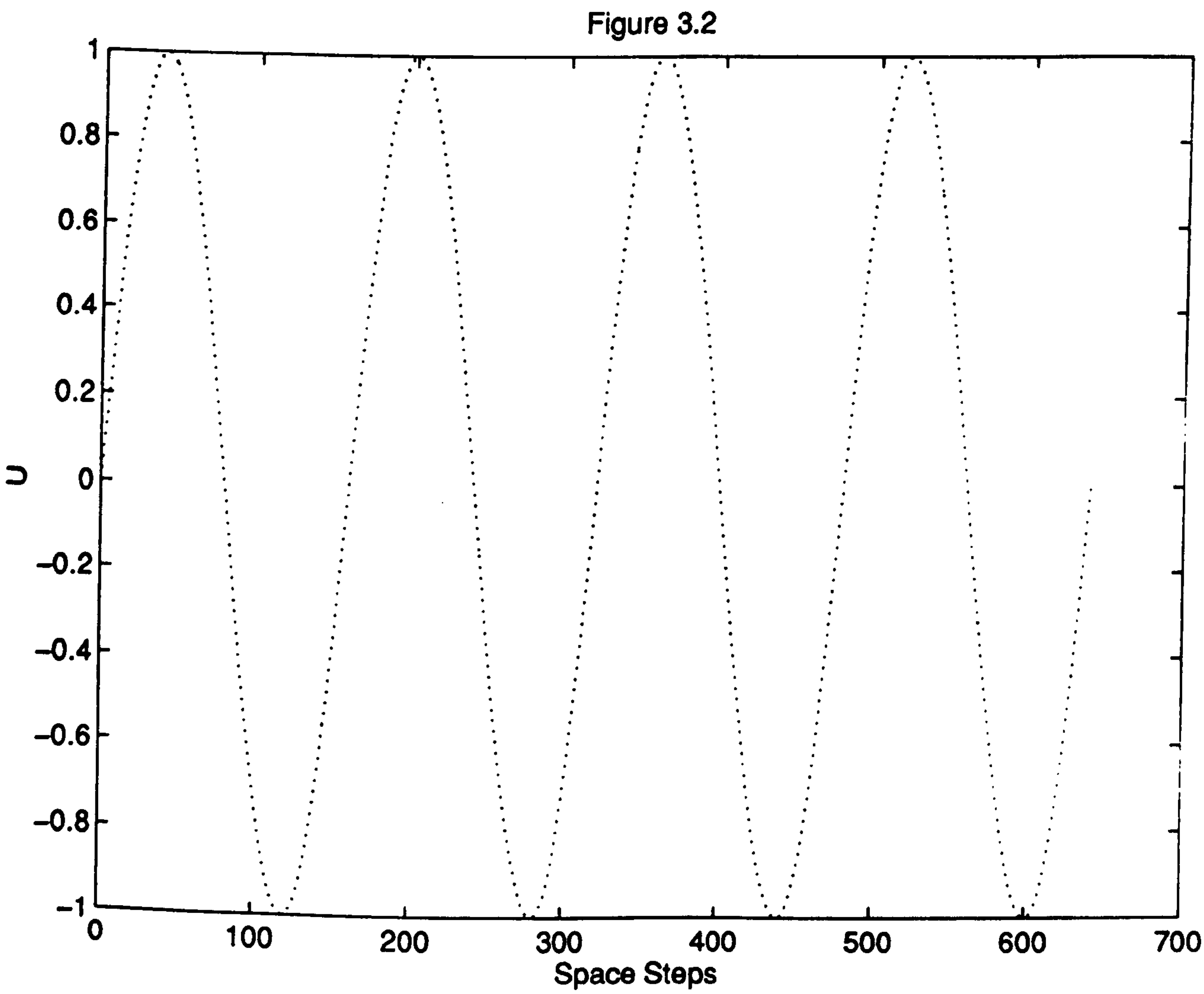

Figure 3.2: Numerical solution of example 1 for $k = 4$, $h = \frac{1}{640}$ and $l = \frac{1}{80}$ at time t=10.0

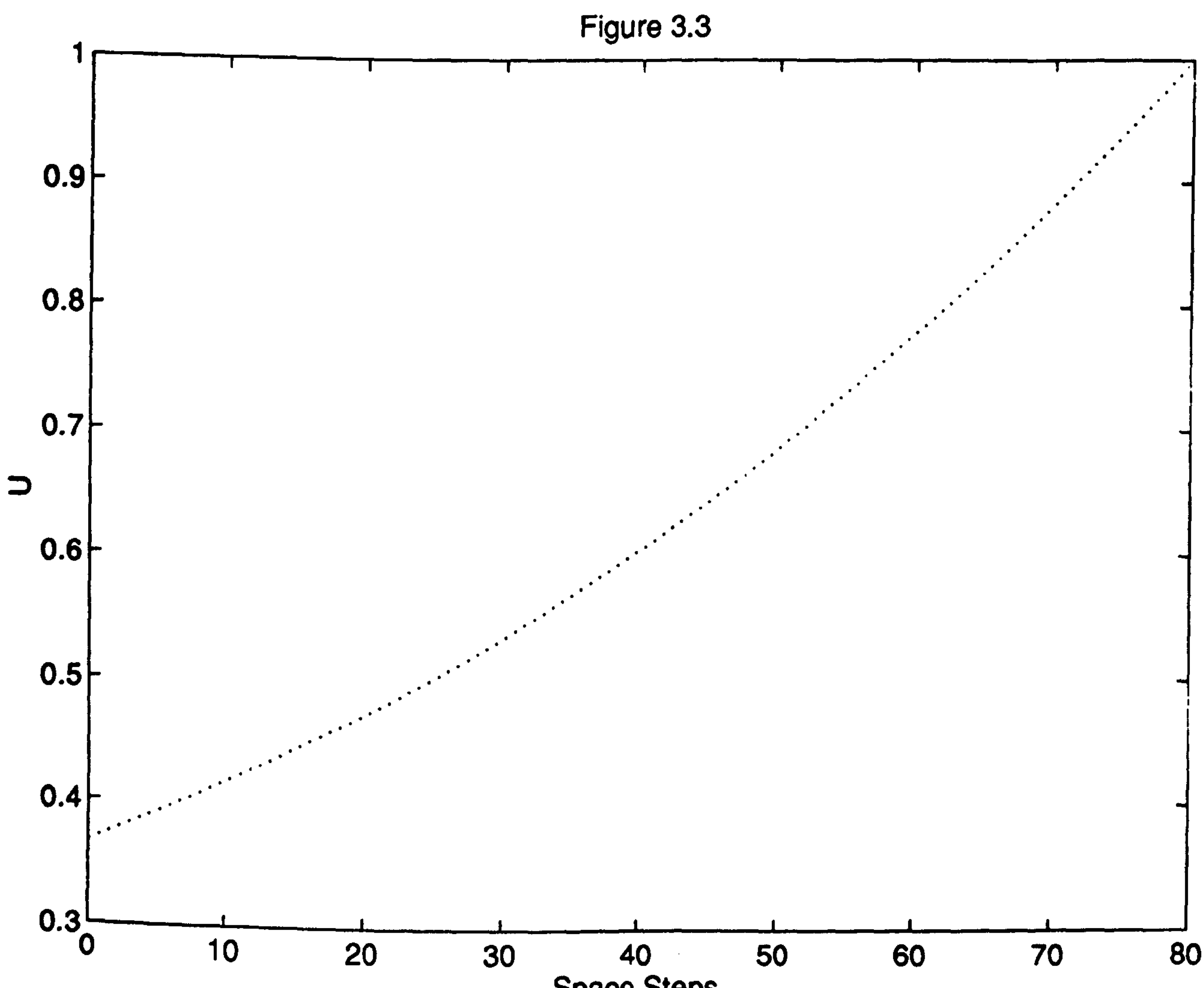

Figure 3.3: Numerical solution of example 2 for $h = \frac{1}{80}$ and $l = \frac{1}{120}$ at time t=1.0

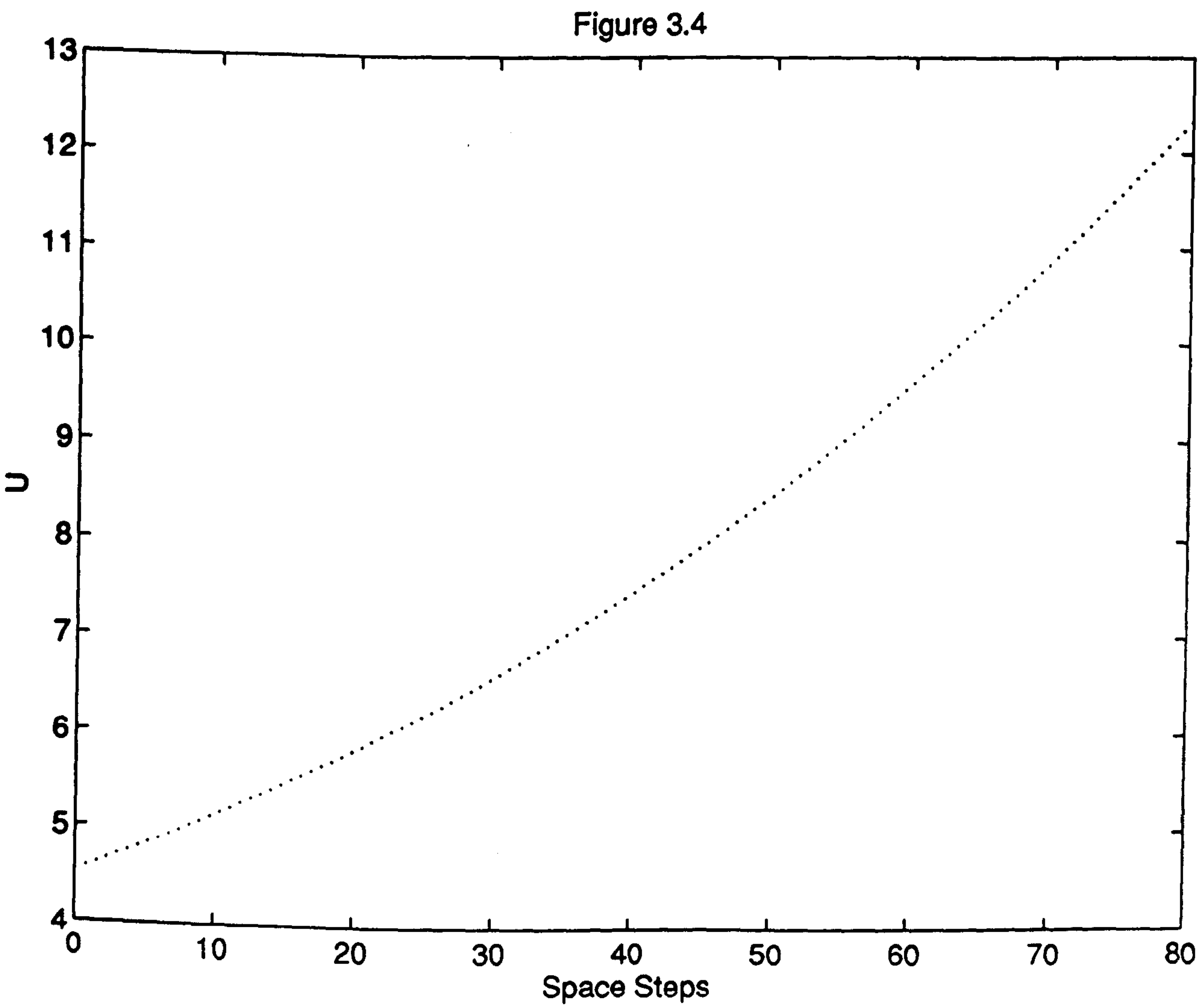

Figure 3.4: Numerical solution of example 2 for $h = \frac{1}{80}$ and $l = \frac{1}{120}$ at time t=10.0

Chapter 4

Third-Order Methods for the Advection-Diffusion Equation

4.1 The Model Problem

A typical problem in applied mathematics is the advection-diffusion equation. This initial/ boundary-value problem (IBVP) is given by

$$\frac{\partial u(x,t)}{\partial t} + \alpha \frac{\partial u(x,t)}{\partial x} = \beta \frac{\partial^2 u}{\partial x^2} + f(x,t), \quad \alpha, \beta > 0, \ 0 < x < X, \ t > 0 \qquad (4.1)$$

with the boundary conditions

$$u(0,t) = h_1(t), \quad t > 0 \qquad (4.2)$$

$$u(X,t) = h_2(t), \quad t > 0 \qquad (4.3)$$

and the initial condition

$$u(x,0) = g(x), \quad 0 \le x \le X \qquad (4.4)$$

where $g(x)$ is a given continuous function of x and $h_1(t)$, $h_2(t)$ are given continuous functions of t.

4.2 The Method

Dividing the interval $[0, X]$ into $N+1$ subintervals each of width h, so that $(N+1)h = X$, and the time variable t into time steps each of length l gives a rectangular mesh of points with co-ordinates

$$(x_m, t_n) = (mh, nl)$$

($m = 0, 1, 2, \ldots, N+1$ and $n = 0, 1, 2, \ldots$) covering the region $R = [0 < x < X] \times [t > 0]$ and its boundary ∂R consisting of the lines $x = 0$, $x = X$ and $t = 0$.

To approximate the first-order space derivative in (4.1) to third-order accuracy at some general point (x, t) of the mesh, assume that it may be replaced by the four-point formula

$$\begin{aligned} \frac{\partial u(x,t)}{\partial x} &= \frac{1}{h}\{a\,u(x-h,t) + b\,u(x,t) + c\,u(x+h,t) \\ &+ d\,u(x+2h,t)\}. \end{aligned} \qquad (4.5)$$

Expanding the terms $u(x-h,t)$, $u(x+h,t)$ and $u(x+2h,t)$ as Taylor series about (x,t) in (4.5) gives

$$\begin{aligned} h\frac{\partial u(x,t)}{\partial x} &= (a+b+c+d)\,u(x,t) \\ &+ (-a+c+2d)\,h\frac{\partial u(x,t)}{\partial x} \\ &+ \frac{1}{2!}(a+c+4d)\,h^2\frac{\partial^2 u(x,t)}{\partial x^2} \\ &+ \frac{1}{3!}(-a+c+8d)\,h^3\frac{\partial^3 u(x,t)}{\partial x^3} \\ &+ \frac{1}{4!}(a+c+16d)\,h^4\frac{\partial^4 u(x,t)}{\partial x^4} \\ &+ O(h^5) \;\; as \;\; h \to 0. \end{aligned} \qquad (4.6)$$

Equating powers of $h^i (i = 0, 1, 2, 3)$ in (4.6) gives

$$\begin{aligned} a + b + c + d &= 0, \\ -a + c + 2d &= 1, \\ a + c + 4d &= 0, \\ -a + c + 8d &= 0. \end{aligned} \qquad (4.7)$$

The solution of the linear system (4.7) is

$$a = \frac{-1}{3}, \quad b = \frac{-1}{2}, \quad c = 1, \quad d = \frac{-1}{6}. \qquad (4.8)$$

Thus

$$\begin{aligned} \frac{\partial u(x,t)}{\partial x} &= \frac{1}{6h}\{-2u(x-h,t) - 3u(x,t) + 6u(x+h,t) \\ &- u(x+2h,t)\} + \frac{h^3}{12}\frac{\partial^4 u(x,t)}{\partial x^4} + O(h^4) \quad as \quad h \to 0 \end{aligned} \qquad (4.9)$$

is the desired third-order approximation to the first-order space derivative at (x, t).

Equation (4.9) is valid only for $(x, t) = (x_m, t_n)$ with $m = 1, 2, \ldots, N - 1$. To attain the same accuracy at the end point (x_N, t_n), a special formula must be developed which approximates $\partial u(x,t)/\partial x$ not only to third order but also with dominant error term $\frac{1}{12}h^3 \partial^4 u(x,t)/\partial x^4$ for $x = x_N$ and $t = t_n$. To achieve this, a five-point formula will be needed. Consider, then, the approximation to $\partial u(x,t)/\partial x$ at the point $(x, t) = (x_N, t_n)$: let

$$\begin{aligned} 6h\frac{\partial u(x,t)}{\partial x} &= a\,u(x-3h,t) + b\,u(x-2h,t) + c\,u(x-h,t) \\ &+ d\,u(x,t) + e\,u(x+h,t) + \frac{1}{2}h^4\frac{\partial^4 u(x,t)}{\partial x^4} \\ &+ O(h^5) \quad as \quad h \to 0. \end{aligned} \qquad (4.10)$$

Then expanding the terms $u(x-3h,t)$, $u(x-2h,t)$, $u(x-h,t)$ and $u(x+h,t)$ as Taylor series about the point (x,t) gives

$$\begin{aligned} 6h\frac{\partial u(x,t)}{\partial x} &= (a+b+c+d+e)\,u(x,t) \\ &+ (-3a-2b-c+e)\,h\frac{\partial u(x,t)}{\partial x} \\ &+ \frac{1}{2!}(9a++4b+c+e)\,h^2\frac{\partial^2 u(x,t)}{\partial x^2} \\ &+ \frac{1}{3!}(-27a-8b-c+e)\,h^3\frac{\partial^3 u(x,t)}{\partial x^3} \\ &+ \frac{1}{4!}(81a++16b+c+e-12)\,h^4\frac{\partial^4 u(x,t)}{\partial x^4} \\ &+ O(h^5) \;\; as \;\; h\to 0. \end{aligned} \tag{4. 11}$$

Equating powers of $h^i (i=0,1,2,3,4)$ in (4.11) gives

$$\begin{aligned} a+b+c+d+e &= 0, \\ -3a-2b-c+e &= 6, \\ 9a+4b+c+e &= 0, \\ -27a-8b-c+e &= 0, \\ 81a+16b+c+e &= -12. \end{aligned} \tag{4. 12}$$

The solution of the linear system (4.12) is

$$a=-1, \quad b=5, \quad c=-12, \quad d=7, \quad e=1. \tag{4. 13}$$

Thus, at the mesh point (x_N, t_n), the desired approximation to $\frac{\partial u(x,t)}{\partial x}$ is

$$\begin{aligned} \frac{\partial u(x,t)}{\partial x} &= \frac{1}{6h}\{-u(x-3h,t)+5u(x-2h,t)-12\,u(x-h,t)+7u(x,t) \\ &+ u(x+h,t)\}+\frac{h^3}{12}\frac{\partial^4 u(x,t)}{\partial x^4}+O(h^4) \;\; as \;\; h\to 0. \end{aligned} \tag{4. 14}$$

Third-order approximations to the second-order space derivative in (4.1) (introduced in [38]) are given by

$$\frac{\partial^2 u(x,t)}{\partial x^2} = \frac{1}{12h^2}\{11u(x-h,t)-20u(x,t)+6\,u(x+h,t)+4u(x+2h,t)$$

$$- \quad u(x+3h,t)\} + \frac{h^3}{12}\frac{\partial^5 u(x,t)}{\partial x^5} + O(h^4) \quad as \quad h \to 0. \qquad (4.15)$$

for $(x,t) = (x_m, t_n), \quad m = 1, 2, \ldots, N-2,$

$$\begin{aligned} \frac{\partial^2 u(x,t)}{\partial x^2} &= \frac{1}{12h^2}\{u(x-3h,t) - 6u(x-2h,t) + 26\,u(x-h,t) \\ &- 40u(x,t) + 21u(x+h,t) - 2u(x+2h,t)\} \\ &+ \frac{h^3}{12}\frac{\partial^5 u(x,t)}{\partial x^5} + O(h^4) \quad as \quad h \to 0. \end{aligned} \qquad (4.16)$$

for $(x,t) = (x_{N-1}, t_n)$ and

$$\begin{aligned} \frac{\partial^2 u(x,t)}{\partial x^2} &= \frac{1}{12h^2}\{2u(x-4h,t) - 11u(x-3h,t) + 24\,u(x-2h,t) \\ &- 14u(x-h,t) - 10u(x,t) + 9u(x+h,t)\} \\ &+ \frac{h^3}{12}\frac{\partial^5 u(x,t)}{\partial x^5} + O(h^4) \quad as \quad h \to 0. \end{aligned} \qquad (4.17)$$

for $(x,t) = (x_N, t_n)$.

Applying (4.1)–(4.4) with (4.9), (4.14), (4.15), (4.16) and (4.17) as appropriate to the N mesh points of the grid at time level $t = t_n$ leads to the system of first-order ordinary differential equations given in vector-matrix form as

$$\frac{d\mathbf{U}(t)}{dt} = A\mathbf{U}(t) + \mathbf{b}(t), \quad t > 0 \qquad (4.18)$$

with initial distribution

$$\mathbf{U}(0) = \mathbf{g}, \qquad (4.19)$$

where

$$\begin{aligned} \mathbf{U}(t) &= [U_1(t), \ldots, U_N(t)]^T, \\ \mathbf{b}(t) &= [f_1(t) + \frac{1}{12h^2}(4\alpha h + 11\beta)h_1(t), f_2(t), f_3(t), \ldots, f_{N-3}(t), \\ &\quad f_{N-2}(t) - \frac{\beta}{12h^2}h_2(t), f_{N-1}(t) + \frac{1}{12h^2}(2\alpha h - 2\beta)h_2(t), \\ &\quad f_N(t) + \frac{1}{12h^2}(-2\alpha h + 9\beta)h_2(t)]^T, \\ \mathbf{g} &= [g(x_1), g(x_2), \ldots, g(x_N)]^T, \end{aligned}$$

T denoting transpose and

$$A = \frac{1}{12h^2}\begin{bmatrix} a_2 & a_3 & a_4 & a_5 & & & & \bigcirc \\ a_1 & a_2 & a_3 & a_4 & a_5 & & & \\ & a_1 & a_2 & a_3 & a_4 & a_5 & & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & & a_1 & a_2 & a_3 & a_4 & a_5 \\ & & & & a_1 & a_2 & a_3 & a_4 \\ & & & a_6 & a_7 & a_8 & a_9 & a_{10} \\ \bigcirc & & & a_{11} & a_{12} & a_{13} & a_{14} & a_{15} \end{bmatrix}_{N\times N} \qquad (4.20)$$

in which

$$\begin{array}{lll} a_1 = 4\alpha h + 11\beta, & a_2 = 4\alpha h + 11\beta, & a_3 = -12\alpha h + 6\beta, \\ a_4 = 2\alpha h + 4\beta, & a_5 = -\beta, & a_6 = \beta, \\ a_7 = -6\beta, & a_8 = 4\alpha h + 26\beta, & a_9 = 6\alpha h - 40\beta, \\ a_{10} = -12\alpha h + 21\beta, & a_{11} = 2\beta, & a_{12} = 2\alpha h - 11\beta, \\ a_{13} = -10\alpha h + 24\beta, & a_{14} = 24\alpha h - 14\beta, & a_{15} = -14\alpha h - 10\beta. \end{array}$$

Solving (4.18) subject to (4.19) gives the solution

$$\mathbf{U}(t) = exp(tA)\mathbf{U}(0) + \int_0^t exp[(t-s)A]\mathbf{b}(s)ds \qquad (4.21)$$

which satisfies the recurrence relation

$$\mathbf{U}(t+l) = exp(lA)\mathbf{U}(t) + \int_t^{t+l} exp[(t+l-s)A]\mathbf{b}(s)ds. \qquad (4.22)$$

Approximating the matrix exponential function $exp(lA)$ in (4.22) by

$$exp(lA) = D^{-1}N \qquad (4.23)$$

in which

$$D = I - a_1 lA + a_2 l^2 A^2 - (\frac{1}{6} - \frac{1}{2}a_1 + a_2)l^3 A^3 \qquad (4.24)$$

is non-singular and

$$N = I + (1 - a_1)lA + (\frac{1}{2} - a_1 + a_2)l^2 A^2 \qquad (4.25)$$

as in Chapter 2 and the integral term by

$$\int_t^{t+l} exp((t+l-s)A)\mathbf{b}(s)ds = W_1\mathbf{b}(s_1) + W_2\mathbf{b}(s_2) + W_3\mathbf{b}(s_3) \qquad (4.\ 26)$$

where $s_1 \neq s_2 \neq s_3$ and W_1, W_2 and W_3 are matrices.

These matrices can be obtained by putting $\lambda = -1$ in (2.53)-(2.55) giving

$$W_1 = \frac{l}{6}\{(I + (4 - 9a_1 + 12a_2)lA\} D^{-1}, \qquad (4.\ 27)$$

$$W_2 = \frac{2l}{3}\{(I - (1 - 3a_1 + 6a_2)lA\} D^{-1}, \qquad (4.\ 28)$$

$$W_3 = \frac{l}{6}\{(I + (3 - 9a_1 + 12a_2)lA + (1 - 3a_1 + 6a_2)l^2A^2\} D^{-1}. \qquad (4.\ 29)$$

Hence (4.22) can be written as

$$\mathbf{U}(t+l) = exp(lA)\mathbf{U}(t) + W_1\mathbf{b}(t) + W_2\mathbf{b}(t + \frac{l}{2}) + W_3\mathbf{b}(t+l). \qquad (4.\ 30)$$

4.3 Algorithm

The algorithm is very similar to that given in Section 2.4 of Chapter 2 but it is included in the interests of completeness.

Assuming that r_1, r_2 and r_3 are the real zeros of

$$q(\theta) = 1 - a_1\theta + a_2\theta^2 - (\frac{1}{6} - \frac{a_1}{2} + a_2)\theta^3 \qquad (4.\ 31)$$

then D given by (4.24) can be factorized as

$$D = (I - \frac{l}{r_1}A)(I - \frac{l}{r_2}A)(I - \frac{l}{r_3}A) \qquad (4.\ 32)$$

and then (4.54) can be written in partial fraction form as

$$\mathbf{U}(t+l) = \left\{c_{11}(I - \frac{l}{r_1}A)^{-1} + c_{12}(I - \frac{l}{r_2}A)^{-1} + c_{13}(I - \frac{\lambda l}{r_3}A)^{-1}\right\}\mathbf{U}(t)$$

$$
\begin{aligned}
&+ \frac{l}{6}\left\{c_{21}(I-\frac{l}{r_1}A)^{-1}+c_{22}(I-\frac{l}{r_2}A)^{-1}+c_{23}(I-\frac{l}{r_3}A)^{-1}\right\}\mathbf{b}(t)\\
&+ \frac{2l}{3}\left\{c_{31}(I-\frac{l}{r_1}A)^{-1}+c_{32}(I-\frac{l}{r_2}A)^{-1}+c_{33}(I-\frac{l}{r_3}A)^{-1}\right\}\mathbf{b}(t+\frac{l}{2})\\
&+ \frac{l}{6}\left\{c_{41}(I-\frac{l}{r_1}A)^{-1}+c_{42}(I-\frac{l}{r_2}A)^{-1}+c_{43}(I-\frac{l}{r_3}A)^{-1}\right\}\mathbf{b}(t+l)
\end{aligned}
\tag{4. 33}
$$

where

$$c_{1j} = \frac{1+(1-a_1)r_j+(\frac{1}{2}-a_1+a_2)r_j^2}{\prod^3_{\substack{i=1\\ i\neq j}}(1-\frac{r_j}{r_i})}, \quad j=1,2,3,$$

$$c_{2j} = \frac{1+(4-9a_1+12a_2)r_j}{\prod^3_{\substack{i=1\\ i\neq j}}(1-\frac{r_j}{r_i})}, \quad j=1,2,3,$$

$$c_{3j} = \frac{1-(1-3a_1+6a_2)r_j}{\prod^3_{\substack{i=1\\ i\neq j}}(1-\frac{r_j}{r_i})}, \quad j=1,2,3$$

and

$$c_{4j} = \frac{1+(3-9a_1+12a_2)r_j+(1-3a_1+6a_2)r_j^2}{\prod^3_{\substack{i=1\\ i\neq j}}(1-\frac{r_j}{r_i})}, \quad j=1,2,3.$$

So that

$$
\begin{aligned}
\mathbf{U}(t+l) &= A_1^{-1}\{c_{11}\mathbf{U}(t)+\frac{l}{6}(c_{21}\mathbf{b}(t)+4c_{31}\mathbf{b}(t+\frac{l}{2})+c_{41}\mathbf{b}(t+l))\}\\
&+ A_2^{-1}\{c_{12}\mathbf{U}(t)+\frac{l}{6}(c_{22}\mathbf{b}(t)+4c_{32}\mathbf{b}(t+\frac{l}{2})+c_{42}\mathbf{b}(t+l))\}\\
&+ A_3^{-1}\{c_{13}\mathbf{U}(t)+\frac{l}{6}(c_{23}\mathbf{b}(t)+4c_{33}\mathbf{b}(t+\frac{l}{2})+c_{43}\mathbf{b}(t+l))\},
\end{aligned}
\tag{4. 34}
$$

where

$$A_i = I-\frac{l}{r_i}A, \quad i=1,2,3, \tag{4. 35}$$

or

$$\mathbf{U}(t+l) = \sum_{i=1}^{3} A_i^{-1}\mathbf{z}_i \qquad (4.36)$$

where

$$\mathbf{z}_i = c_{1i}\mathbf{U}(t) + \frac{l}{6}\{c_{2i}\mathbf{b}(t) + 4c_{3i}\mathbf{b}(t+\frac{l}{2}) + c_{4i}\mathbf{b}(t+l)\}, \quad i = 1,2,3.$$

Let

$$A_i^{-1}\mathbf{z}_i = \mathbf{y}_i$$

then

$$\mathbf{U}(t+l) = \mathbf{y}_1 + \mathbf{y}_2 + \mathbf{y}_3 \qquad (4.37)$$

in which $\mathbf{y}_1$, $\mathbf{y}_2$ and $\mathbf{y}_3$ are the solutions of the systems

$$A_i\mathbf{y}_i = \mathbf{z}_i, \quad i = 1,2,3. \qquad (4.38)$$

respectively. This algorithm is presented in tabular form in Table 4.1.

4.4 Numerical Example

In this section only a representative of many other methods based on (4.23) will be used. So taking

$$a_1 = \frac{65431}{50000}$$

and

$$a_2 = \frac{171151}{300000},$$

as in chapter 2, gives

$$r_1 = 2.18837132239026, \quad r_2 = 2.33987492247039, \quad r_3 = 2.35690139372652$$

as the real zeros of (4.55). These values produce

$$c_{11} = -176.185066638, \quad c_{12} = 2051.11129521, \quad c_{13} = -1873.92622858,$$

$c_{21} = -224.317807049, \quad c_{22} = 2358.75587416, \quad c_{23} = -2133.43806711,$

$c_{31} = -19.0008161810, \quad c_{32} = 326.498892802, \quad c_{33} = -306.498076621,$

$c_{41} = -182.736963963, \quad c_{42} = 1594.78928297, \quad c_{43} = -1411.05231901$

By the way of an example consider the one space variable partial differential equation

$$\frac{\partial u}{\partial t} + 5\frac{\partial u}{\partial x} = \beta\frac{\partial^2 u}{\partial x^2}, \quad 0 < x < 1, \quad t > 0. \tag{4. 39}$$

subject to the boundary conditions

$$h_1(t) = u(0,t) = \sqrt{\frac{2}{2+\beta t}}\ exp\left(\frac{-(2+5t)^2}{4(2+\beta t)}\right), \quad t > 0, \tag{4. 40}$$

$$h_2(t) = u(1,t) = \sqrt{\frac{2}{2+\beta t}}\ exp\left(\frac{-(1+5t)^2}{4(2+\beta t)}\right), \quad t > 0, \tag{4. 41}$$

and the initial condition

$$g(x) = u(x,0) = exp\left(\frac{-(x-2)^2}{8}\right), \quad t > 0. \tag{4. 42}$$

This problem has theoretical solution

$$u(x,t) = \sqrt{\frac{2}{2+\beta t}}\ exp\left(\frac{-(x-2-5t)^2}{4(2+\beta t)}\right), \tag{4. 43}$$

(see Jain *et al.* [19]). Using the algorithm developed in Section 4.3 with the information given at the beginning of this section the problem {(4.63)-(4.66)} was solved for $h = 0.1, 0.05, 0.005, 0.001$ and $l = 0.1, 0.05, 0.005, 0.001$ using $\beta = 1000$. In these experiments the method behaves smoothly over the whole interval $0 \le x \le 1$ and no contrived oscillations are observed. The maximum errors at time t=0.5 are observed at mid point of the region and are given in Table 4.2. For pictorial evidence of stability, accuracy and smoothness of the method the theoretical and numerical solutions for $h = 0.1$ and $l = 0.1$ at time $t = 0.5$ are depicted in Figure 4.1 and Figure 4.2 respectively.

Table 4.1: Algorithm 1

Steps	Processor 1	Processor 2	Processor 3
1 Input	$l, r_1, \mathbf{U}_0, A$ $c_{11}, c_{21}, c_{31}, c_{41}$	$l, r_2, \mathbf{U}_0, A$ $c_{12}, c_{22}, c_{32}, c_{42}$	$l, r_3, \mathbf{U}_0, A$ $c_{13}, c_{23}, c_{33}, c_{43}$
2 Compute	$I - \frac{l}{r_1}A$	$I - \frac{l}{r_2}A$	$I - \frac{l}{r_3}A$
3 Decompose	$I - \frac{l}{r_1}A = L_1U_1$	$I - \frac{l}{r_2}A = L_2U_2$	$I - \frac{l}{r_3}A = L_3U_3$
4 Evaluate	$\mathbf{b}(t)$, $\mathbf{b}(t+\frac{l}{2})$ $\mathbf{b}(t+l)$	$\mathbf{b}(t)$, $\mathbf{b}(t+\frac{l}{2})$ $\mathbf{b}(t+l)$	$\mathbf{b}(t)$, $\mathbf{b}(t+\frac{l}{2})$ $\mathbf{b}(t+l)$
5 Using	$\mathbf{w}_1(t) = \frac{l}{6}(c_{21}\mathbf{b}(t)$ $+4c_{31}\mathbf{b}(t+\frac{l}{2})$ $+c_{41}\mathbf{b}(t+l))$	$\mathbf{w}_2(t) = \frac{l}{6}(c_{22}\mathbf{b}(t)$ $+4c_{32}\mathbf{b}(t+\frac{l}{2})$ $+c_{42}\mathbf{b}(t+l))$	$\mathbf{w}_3(t) = \frac{l}{6}(c_{23}\mathbf{b}(t)$ $+4c_{33}\mathbf{b}(t+\frac{l}{2})$ $+c_{43}\mathbf{b}(t+l))$
6 Solve	$L_1U_1\mathbf{y}_1(t)$ $= c_{11}\mathbf{U}(t) + \mathbf{w}_1(t)$	$L_2U_2\mathbf{y}_2(t)$ $= c_{12}\mathbf{U}(t) + \mathbf{w}_2(t)$	$L_3U_3\mathbf{y}_3(t)$ $= c_{13}\mathbf{U}(t) + \mathbf{w}_3(t)$
7	$\mathbf{U}(t+l) = \mathbf{y}_1(t) + \mathbf{y}_2(t) + \mathbf{y}_3(t)$		
8	GO TO Step 4 for next time step		

Table 4.2: Maximum errors for Example 1 at $t = 0.5$

h	0.1	0.05	0.005	0.001
$l = 0.1$	0.1270D-6	0.1270D-6	0.1270D-6	0.1270D-6
$l = 0.05$	0.2746D-7	0.2746D-7	0.2744D-7	0.2747D-7
$l = 0.005$	0.1192D-8	0.1192D-8	0.1182D-8	0.1189D-8
$l = 0.001$	0.4805D-9	0.4806D-9	0.4716D-9	0.4752D-9

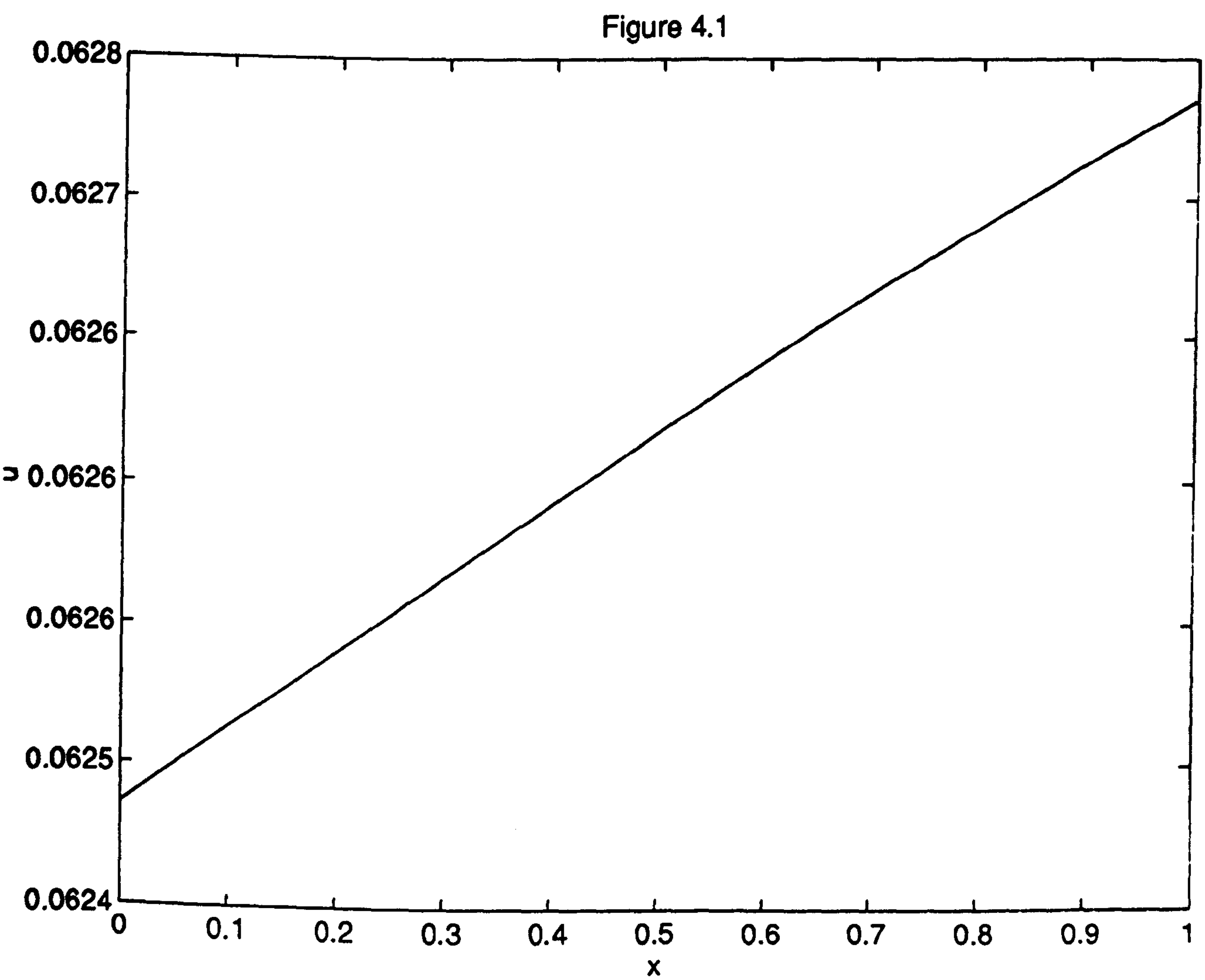

Figure 4.1: Theoretical solution of example 1 for time t=0.5

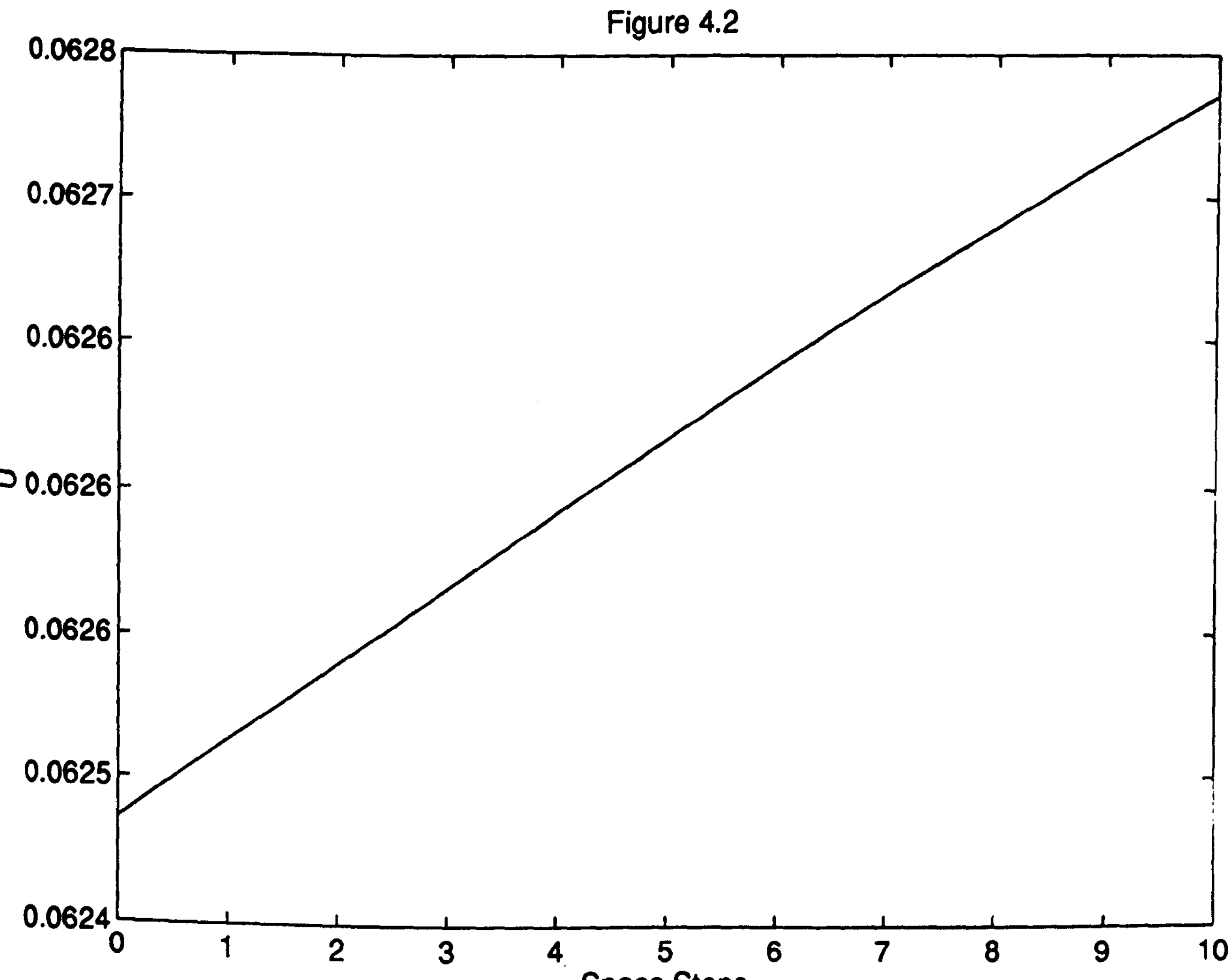

Figure 4.2: Numerical solution of example 1 for $h = 0.1$, and $l = 0.1$ at time t=0.5

Chapter 5

Fourth-Order Numerical Methods for the Advection-Diffusion Equation

To develop fourth-order numerical methods for advection-diffusion equations of the type (4.1) with appropriate initial and boundary conditions specified, the space derivatives in the partial differential equation are replaced by fourth-order finite-difference approximations resulting in a system of first-order ordinary differential equations the solution of which satisfies a recurrence relation. The accuracy in time is controlled by a fourth-order approximation to the matrix exponential function as in Chapter 3.

5.1 The Method

Consider the advection-diffusion equation (4.1), mentioned here for convenience,

$$\frac{\partial u(x,t)}{\partial t} + \alpha\frac{\partial u(x,t)}{\partial x} = \beta\frac{\partial^2 u(x,t)}{\partial x^2} + f(x,t); \quad \alpha,\beta > 0, \quad 0 < x < X, \quad t > 0 \tag{5.1}$$

with the boundary conditions

$$\left.\begin{array}{l} u(0,t) = f_1(t) \\ u(1,t) = f_2(t) \end{array}\right\}, \quad t > 0 \qquad (5.2)$$

in which $f_1(t)$, $f_2(t)$ are given continuous functions of t and the initial condition

$$u(x,0) = g(x), \quad 0 \leq x \leq X, \qquad (5.3)$$

in which $g(x)$ is a given continuous functions of x. For a positive integer N, let $h = \frac{X}{N+1}$. Considering the discretization of the region $R = [0 < x < X] \times [t > 0]$ and its boundary ∂R as in Section 4.2, assume that the combination

$$a\,u(x-2h,t) + b\,u(x-h,t) + c\,u(x,t) + d\,u(x+h,t) + e\,u(x+2h,t)$$

gives the fourth-order approximation to $\frac{\partial u}{\partial x}$ at some general point (x,t) of the mesh. Expanding the terms $u(x-2h,t), u(x-h,t), u(x+h,t)$ and $u(x+2h,t)$ as Taylor series about the point (x,t) gives

$$\begin{aligned} a\,u(x-2h,t) + b\,u(x-h,t) &+ c\,u(x,t) + d\,u(x+h,t) + e\,u(x+2h,t) \\ &= (a+b+c+d+e)u(x,t) \\ &+ (-2a-b+d+2e)h\frac{\partial u}{\partial x} \\ &+ \frac{1}{2!}(4a+b+d+4e)h^2\frac{\partial^2 u}{\partial x^2} \\ &+ \frac{1}{3!}(-8a-b+d+8e)h^3\frac{\partial^3 u}{\partial x^3} \\ &+ \frac{1}{4!}(16a+b+d+16e)h^4\frac{\partial^4 u}{\partial x^4} \\ &+ \frac{1}{5!}(-324a-b+d+32e)h^5\frac{\partial^5 u}{\partial x^5} \\ &+ O(h^6) \;\; as \;\; h \to 0. \qquad (5.4) \end{aligned}$$

Equating the powers of $h^i (i = 0,2,3,4)$ in (5.4) to zero and the power of h to 1 gives

$$c + d + b + e + a \;=\; 0$$

$$
\begin{aligned}
d-b+2e-2a &= 1 \\
d+b+4e+4a &= 0 \\
d-b+8e-8a &= 0 \\
d+b+16e+16a &= 0.
\end{aligned} \qquad (5.5)
$$

Solution of this linear system is

$$
a=\frac{1}{12},\quad b=\frac{-8}{12},\quad c=0,\quad d=\frac{8}{12},\quad e=-\frac{1}{12}.
$$

So that

$$
\begin{aligned}
\frac{1}{12}u(x-2h,t) &- \frac{8}{12}u(x-h,t)+\frac{8}{12}u(x+h,t)-\frac{1}{12}u(x+2h,t) \\
&= h\frac{\partial u}{\partial x}-\frac{1}{30}h^5\frac{\partial^5 u}{\partial x^5}+O(h^6) \quad as \quad h\to 0. \qquad (5.6)
\end{aligned}
$$

Thus the desired approximation to $\frac{\partial u}{\partial x}$ is given by

$$
\begin{aligned}
\frac{\partial u}{\partial x} &= \frac{1}{12h}\{u(x-2h,t)-8u(x-h,t)+8u(x+h,t)-u(x+2,t)\} \\
&+ \frac{1}{30}h^4\frac{\partial^5 u}{\partial x^5}+O(h^5) \quad as \quad h\to 0. \qquad (5.7)
\end{aligned}
$$

It can be noted that equation (5.7) is only valid for $(x,t)=(x_m,t_n)$ with $m=2,3,4,\ldots,N-1$. To attain the same accuracy at the end points (x_1,t_n) and (x_N,t_n) special formulae must be devolped which approximate $\frac{\partial u}{\partial x}$ not only to fourth-order but also with dominant error term $\frac{1}{30}h^4\frac{\partial^5 u}{\partial x^5}$ for $x=x_1,x_N$ and $t=t_n$.

Consider then the approximation to $\frac{\partial u}{\partial x}$ at the point $(x,t)=(x_1,t_n)$; let

$$
\begin{aligned}
12h\frac{\partial u}{\partial x} &= a\,u(x-h,t)+b\,u(x,t)+c\,u(x+h,t)+d\,u(x+2h,t) \\
&+ e\,u(x+3h,t)+\frac{2}{5}h^5\frac{\partial^5 u}{\partial x^5}+O(h^6) \quad as \quad h\to 0. \qquad (5.8)
\end{aligned}
$$

Expanding the terms $u(x-h,t), u(x+h,t), u(x+2h,t)$ and $u(x+3h,t)$ as Taylor series about the point (x,t) gives

$$
\begin{aligned}
12h\frac{\partial u}{\partial x} &= (a+b+c+d+e)u(x,t) \\
&+ (-a+c+2d+3e)h\frac{\partial u}{\partial x} \\
&+ \frac{1}{2}(a+c+4d+9e)h^2\frac{\partial^2 u}{\partial x^2} \\
&+ \frac{1}{6}(-a+c+8d+27e)h^3\frac{\partial^3 u}{\partial x^3} \\
&+ \frac{1}{24}(a+c+16d+81e)h^4\frac{\partial^4 u}{\partial x^4} \\
&+ \frac{1}{120}(-a+c+32d+243e)h^5\frac{\partial^5 u}{\partial x^5} \\
&+ O(h^6) \;\; as \;\; h \to 0. \qquad (5.\ 9)
\end{aligned}
$$

Equating the powers of $h^i (i = 0,1,2,3,4)$ in (5.9) gives

$$
\begin{aligned}
b+a+c+d+e &= 0 \\
-a+c+2d+3e &= 12 \\
a+c+4d+9e &= 0 \qquad (5.\ 10) \\
-a+c+8d+27e &= 0 \\
a+c+16d+81e &= 0
\end{aligned}
$$

Solution of the linear system (5.10) is

$$a = -3, \quad b = -10, \quad c = 18, \quad d = -6, \quad e = 1.$$

Thus

$$
\begin{aligned}
\frac{\partial u(x,t)}{\partial x} &= \frac{1}{12h}\{-3u(x-h,t) - 10u(x,t) \\
&+ 18u(x+h,t) - 6u(x+2h,t) + u(x+3h,t)\} \\
&- \frac{1}{20}h^4\frac{\partial^5 u}{\partial x^5} + O(h^5) \;\; as \;\; h \to 0. \qquad (5.\ 11)
\end{aligned}
$$

Consider, now the approximation to $\frac{\partial u(x,t)}{\partial x}$ at the point $(x,t) = (x_N, t_n)$; let

$$\begin{aligned} 12h\frac{\partial u}{\partial x} &= a\,u(x-3h,t) + b\,u(x-2h,t) + c\,u(x-h,t) + d\,u(x,t) \\ &+ \; e\,u(x+h,t) + \frac{12}{5}h^5\frac{\partial^5 u}{\partial x^5} + O(h^6) \;\; as \;\; h \to 0. \end{aligned} \tag{5.12}$$

Expanding the terms $u(x-3h,t), u(x-2h,t), u(x-h,t)$ and $u(x+h,t)$ about the point (x,t) gives

$$\begin{aligned} 12h\frac{\partial u}{\partial x} &= (a+b+c+d+e)u(x,t) \\ &+ (-3a-2b-c+e)h\frac{\partial u}{\partial x} \\ &+ \frac{1}{2}(9a+4b+c+e)h^2\frac{\partial^2 u}{\partial x^2} \\ &+ \frac{1}{6}(-27a-8b-c+e)h^3\frac{\partial^3 u}{\partial x^3} \\ &+ \frac{1}{24}(81a+16b+c+e)h^4\frac{\partial^4 u}{\partial x^4} \\ &+ \frac{1}{120}(-243a-32b-c+e)h^5\frac{\partial^5 u}{\partial x^5} \\ &+ O(h^6) \;\; as \;\; h \to 0. \end{aligned} \tag{5.13}$$

Equating the powers of $h^i (i = 0,1,2,3,4)$ in (5.13) gives

$$\begin{aligned} a+b+c+d+e &= 0 \\ -3a-2b-c+e &= 12 \\ 9a+4b+c+e &= 0 \\ -27a-8b-c+e &= 0 \\ 81a+16b+c+e &= 0. \end{aligned} \tag{5.14}$$

Solving the linear system (5.14) gives

$$a = -1, \quad b = 6, \quad c = -18, \quad d = 10, \quad e = 3.$$

Thus

$$\begin{aligned}\frac{\partial u(x,t)}{\partial x} &= \frac{1}{12h}\{-u(x-3h,t)+6u(x-2h,t)\\ &- 18u(x-h,t)+10u(x,t)+3u(x+h,t)\}\\ &+ \frac{1}{20}h^4\frac{\partial^5 u}{\partial x^5}+O(h^5) \;\; as \;\; h\to 0. \qquad (5.15)\end{aligned}$$

is the desired approximation to $\frac{\partial u(x,t)}{\partial x}$ at the point (x_N, t_n).

Consider, next the fourth-order approximations to $\frac{\partial^2 u(x,t)}{\partial x^2}$ [39];

$$\begin{aligned}\frac{\partial^2 u(x,t)}{\partial x^2} &= \frac{1}{12h^2}\{-u(x-2h,t)+16u(x-h,t)\\ &- 30u(x,t)+16u(x+h,t)-u(x+2h,t)\}\\ &+ \frac{1}{90}h^4\frac{\partial^6 u}{\partial x^6}+O(h^5) \;\; as \;\; h\to 0. \qquad (5.16)\end{aligned}$$

valid for points $(x,t)=(mh,nl)$ $m=2,3,4,\ldots,N-1$,

$$\begin{aligned}\frac{\partial^2 u(x,t)}{\partial x^2} &= \frac{1}{12h^2}\{9u(x-h,t)-9u(x,t)-19u(x+h,t)\\ &+ 34u(x+2h,t)-21u(x+3h,t)+7u(x+4h,t)\\ &- u(x+5h,t)\}+\frac{1}{90}h^4\frac{\partial^6 u}{\partial x^6}+O(h^5) \;\; as \;\; h\to 0. \qquad (5.17)\end{aligned}$$

the approximation to $\frac{\partial^2 u(x,t)}{\partial x^2}$ at the point (x_1, t_n) and

$$\begin{aligned}\frac{\partial^2 u(x,t)}{\partial x^2} &= \frac{1}{12h^2}\{-u(x-5h,t)+7u(x-4h,t)-21u(x-3h,t)\\ &+ 34u(x-2h,t)-19u(x-h,t)\\ &- 9u(x,t)+9u(x+h,t)\}\\ &+ \frac{1}{90}h^4\frac{\partial^6 u}{\partial x^6}+O(h^5) \;\; as \;\; h\to 0. \qquad (5.18)\end{aligned}$$

the approximation to $\frac{\partial^2 u(x,t)}{\partial x^2}$ at the point (x_N, t_n).

Applying (5.1) with (5.7) or (5.11) or (5.16) or (5.17) or (5.18) as appropriate to the N mesh points at the time level $t = nl$, leads to the system of first-order ordinary differential equations given by vector-matrix form as

$$\frac{d\mathbf{U}(t)}{dt} = A\mathbf{U}(t) + \mathbf{b}(t), \quad t > 0 \qquad (5.19)$$

with initial distribution

$$\mathbf{U}(0) = \mathbf{g} \qquad (5.20)$$

in which

$$\begin{aligned} \mathbf{U}(t) &= [U_1(t),\ U_2(t)\ldots,U_N(t)]^T, \\ \mathbf{b}(t) &= [f_1(t) + \tfrac{1}{12h^2}(9\beta + 3\alpha h),\ f_2(t) - \tfrac{1}{12h^2}(\beta + \alpha h),\ f_3(t),\ldots, \\ &\quad f_{N-2},\ f_{N-1}(t) - \tfrac{1}{12h^2}(\beta - \alpha h),\ f_N(t) + \tfrac{1}{12h^2}(9\beta - 3\alpha h)]^T, \\ \mathbf{g} &= [g(x_1),\ g(x_2),\ldots,g(x_N)]^T, \end{aligned}$$

T denoting transpose and

$$A = \frac{1}{12h^2}\begin{bmatrix} a_1 & a_2 & a_3 & a_4 & a_5 & a_6 & \bigcirc \\ a_8 & a_9 & a_{10} & a_{11} & & & \\ a_7 & a_8 & a_9 & a_{10} & a_{11} & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & a_7 & a_8 & a_9 & a_{10} & a_{11} \\ & & & a_7 & a_8 & a_9 & a_{10} \\ \bigcirc & a_6 & a_5 & a_4 & a_3 & a_2 & a_1 \end{bmatrix}_{N\times N} \qquad (5.21)$$

where

$a_1 = -9\beta + 10\alpha h$	$a_2 = -19\beta - 18\alpha h$	$a_3 = 34\beta + 6\alpha h$
$a_4 = -21\beta - \alpha h$	$a_5 = 7\beta$	$a_6 = -\beta$
$a_7 = -\beta - \alpha h$	$a_8 = 16\beta + 8\alpha h$	$a_9 = -30\beta$
$a_{10} = 16\beta - 8\alpha h$	$a_{11} = -\beta + \alpha h$	

Solving (5.19) subject to (5.20) gives the solution

$$\mathbf{U}(t) = exp(tA)\mathbf{U}(0) + \int_0^t exp[(t-s)A]\mathbf{b}(s)ds \qquad (5.22)$$

which satisfies the recurrence relation

$$\mathbf{U}(t+l) = exp(lA)\mathbf{U}(t) + \int_t^{t+l} exp[(t+l-s)A]\mathbf{b}(s)ds. \qquad (5.23)$$

Approximating the matrix exponential function $exp(lA)$ in (5.23) by

$$exp(lA) = D^{-1}N \quad (5.24)$$

where

$$D = I - a_1 lA + a_2 l^2 A^2 - a_3 l^3 A^3 + (\frac{-1}{24} + \frac{1}{6}a_1 - \frac{1}{2}a_2 + a_3) l^4 A^4 \quad (5.25)$$

is a non-singular matrix and

$$N = I + (1 - a_1) lA + (\frac{1}{2} - a_1 + a_2) l^2 A^2 + (\frac{1}{6} - \frac{1}{2}a_1 + a_2 - a_3) l^3 A^3 \quad (5.26)$$

as in Chapter 3 and the integral term by

$$\int_t^{t+l} exp((t + l - s)A)\mathbf{b}(s)ds = W_1\mathbf{b}(s_1) + W_2\mathbf{b}(s_2) + W_3\mathbf{b}(s_3) + W_4\mathbf{b}(s_4) \quad (5.27)$$

where $s_1 \neq s_2 \neq s_3 \neq s_4$ and W_1, W_2, W_3 and W_4 are matrices.

These matrices can be obtained by putting $\lambda = -1$ in (3.63)-(3.66) to give

$$\begin{aligned} W_1 &= \frac{l}{24}\{(3I + (-19 + 78a_1 - 216a_2 + 324a_3)lA \\ &\quad +(3 - 8a_1 + 12a_2)(lA)^2\}\, D^{-1}, \quad (5.28) \\ W_2 &= \frac{3}{16}l\{(2I - (-16 + 56a_1 - 144a_2 + 216a_3)lA \\ &\quad +(1 - 4a_1 + 12a_2 - 24a_3)(lA)^2\}\, D^{-1}, \quad (5.29) \\ W_3 &= \frac{3}{8}l\{(I - (7 - 26a_1 + 72a_2 - 108a_3)lA \\ &\quad -(1 - 4a_1 + 12a_2 - 24a_3)(lA)^2\}\, D^{-1}, \quad (5.30) \\ W_4 &= \frac{l}{48}l\{(6I + (44 - 168a_1 + 432a_2 - 648a_3)lA \\ &\quad +(11 - 44a_1 + 132a_2 - 216a_3)(lA)^2 \\ &\quad + (2 - 8a_1 + 24a_2 - 48a_3)(lA)^3\}\, D^{-1}. \quad (5.31) \end{aligned}$$

Hence (5.23) can be written as

$$\mathbf{U}(t+l) = exp(lA)\mathbf{U}(t) + W_1\mathbf{b}(t) + W_2\mathbf{b}(t+\frac{l}{3}) + W_3\mathbf{b}(t+\frac{2}{3}l) + W_4\mathbf{b}(t+l). \quad (5.32)$$

5.2 Algorithm

The algorithm is similar to that detailed in chapter 3 but it is included for completeness. Assuming that r_1, r_2, r_3 and r_4 ($r_i \neq 0$) are the real zeros of

$$q(\theta) = 1 - a_1\theta + a_2\theta^2 - a_3\theta^3 + (-\frac{1}{24} + \frac{a_1}{6} - \frac{a_2}{2} + a_3)\theta^4 \quad (5.33)$$

then D given by (5.25) can be factorized as

$$D = (I - \frac{l}{r_1}A)(I - \frac{l}{r_2}A)(I - \frac{l}{r_3}A)(I - \frac{l}{r_4}A) \quad (5.34)$$

and then (5.68) can be written in partial-fraction form as

$$\begin{aligned}
\mathbf{U}(t+l) = & \left\{A_1(I - \frac{l}{r_1}A)^{-1} + A_2(I - \frac{l}{r_2}A)^{-1}\right. \\
& \left. + A_3(I - \frac{l}{r_3}A)^{-1} + A_4(I - \frac{l}{r_4}A)^{-1}\right\}\mathbf{U}(t) \\
+ & \frac{l}{24}\left\{B_1(I - \frac{l}{r_1}A)^{-1} + B_2(I - \frac{l}{r_2}A)^{-1}\right. \\
& \left. + B_3(I - \frac{l}{r_3}A)^{-1} + B_4(I - \frac{l}{r_4}A)^{-1}\right\}\mathbf{b}(t) \\
+ & \frac{3}{16}l\left\{C_1(I - \frac{l}{r_1}A)^{-1} + C_2(I - \frac{l}{r_2}A)^{-1}\right. \\
& \left. + C_3(I - \frac{l}{r_3}A)^{-1} + C_4(I - \frac{l}{r_4}A)^{-1}\right\}\mathbf{b}(t+\frac{l}{3}) \\
+ & \frac{3}{8}l\left\{D_1(I - \frac{l}{r_1}A)^{-1} + D_2(I - \frac{l}{r_2}A)^{-1}\right. \\
& \left. + D_3(I - \frac{l}{r_3}A)^{-1} + D_4(I - \frac{l}{r_4}A)^{-1}\right\}\mathbf{b}(t+\frac{2}{3}l)
\end{aligned}$$

$$+ \quad \frac{l}{48}\left\{E_1(I - \frac{l}{r_1}A)^{-1} + E_2(I - \frac{l}{r_2}A)^{-1} + E_3(I - \frac{l}{r_3}A)^{-1} + E_4(I - \frac{l}{r_4}A)^{-1}\right\} \mathbf{b}(t+l) \quad (5.35)$$

in which for $i = 1, 2, 3, 4$

$$A_i = \frac{1 + p_1 r_i + p_2 r_i^2 + p_3 r_i^3}{\prod_{\substack{j=1 \\ j \neq i}}^{4} (1 - \frac{r_i}{r_j})},$$

$$B_i = \frac{3 + p_4 r_i + p_5 r_i^2}{\prod_{\substack{j=1 \\ j \neq i}}^{4} (1 - \frac{r_i}{r_j})},$$

$$C_i = \frac{2 - p_6 r_i + p_7 r_i^2}{\prod_{\substack{j=1 \\ j \neq i}}^{4} (1 - \frac{r_i}{r_j})},$$

$$D_i = \frac{1 - p_8 r_i - p_9 r_i^2}{\prod_{\substack{j=1 \\ j \neq i}}^{4} (1 - \frac{r_i}{r_j})},$$

$$E_i = \frac{6 + p_{10} r_i + p_{11} r_i^2 + p_{12} r_i^3}{\prod_{\substack{j=1 \\ j \neq i}}^{4} (1 - \frac{r_i}{r_j})}$$

where

$$p_1 = 1 - a_1,$$

$$p_2 = \frac{1}{2} - a_1 + a_2,$$

$$p_3 = \frac{1}{6} - \frac{a_1}{2} + a_2 - a_3,$$

$$p_4 = -19 + 78a_1 - 216a_2 + 324a_3,$$

$$p_5 = 3 - 8a_1 + 12a_2,$$

$$p_6 = -16 + 56a_1 - 144a_2 + 216a_3,$$

$$p_7 = 1 - 4a_1 + 12a_2 - 24a_3,$$

$$p_8 = 7 - 26a_1 + 72a_2 - 108a_3,$$

$$
\begin{aligned}
p_9 &= 1 - 4a_1 + 12a_2 - 24a_3, \\
p_{10} &= 44 - 168a_1 + 432a_2 - 648a_3, \\
p_{11} &= 11 - 44a_1 + 132a_2 - 216a_3, \\
p_{12} &= 2 - 8a_1 + 24a_2 - 48a_3.
\end{aligned}
$$

Hence

$$
\begin{aligned}
\mathbf{U}(t+l) &= (I - \frac{1}{r_1} lA)^{-1} \Big[A_1 \mathbf{U}(t) + \frac{l}{24}(B_1 \mathbf{b}(t) + \frac{3}{16} l C_1 \mathbf{b}(t + \frac{l}{3}) \\
&\quad + \frac{3}{8} l D_1 \mathbf{b}(t + \frac{2}{3} l) + \frac{l}{48} E_1 \mathbf{b}(t+l)) \Big] \\
&+ (I - \frac{1}{r_2} lA)^{-1} \Big[A_2 \mathbf{U}(t) + \frac{l}{24}(B_2 \mathbf{b}(t) + \frac{3}{16} l C_2 \mathbf{b}(t + \frac{l}{3}) \\
&\quad + \frac{3}{8} l D_2 \mathbf{b}(t + \frac{2}{3} l) + \frac{l}{48} E_2 \mathbf{b}(t+l)) \Big] \\
&+ (I - \frac{1}{r_3} lA)^{-1} \Big[A_3 \mathbf{U}(t) + \frac{l}{24}(B_3 \mathbf{b}(t) + \frac{3}{16} l C_3 \mathbf{b}(t + \frac{l}{3}) \\
&\quad + \frac{3}{8} l D_3 \mathbf{b}(t + \frac{2}{3} l) + \frac{l}{48} E_3 \mathbf{b}(t+l)) \Big] \\
&+ (I - \frac{1}{r_4} lA)^{-1} \Big[A_4 \mathbf{U}(t) + \frac{l}{24}(B_4 \mathbf{b}(t) + \frac{3}{16} l C_4 \mathbf{b}(t + \frac{l}{3}) \\
&\quad + \frac{3}{8} l D_4 \mathbf{b}(t + \frac{2}{3} l) + \frac{l}{48} E_4 \mathbf{b}(t+l)) \Big] \qquad (5.36)
\end{aligned}
$$

which gives

$$
\begin{aligned}
\mathbf{U}(t+l) &= (I - \frac{1}{r_1} lA)^{-1} \mathbf{z}_1 + (I - \frac{1}{r_i} lA)^{-1} \mathbf{z}_2 \\
&+ (I - \frac{1}{r_3} lA)^{-1} \mathbf{z}_3 + (I - \frac{1}{r_4} lA)^{-1} \mathbf{z}_4, \qquad (5.37)
\end{aligned}
$$

where

$$
\begin{aligned}
\mathbf{z}_i &= A_i \mathbf{U}(t) + \frac{l}{24}(B_i \mathbf{b}(t) + \frac{3}{16} l C_i \mathbf{b}(t + \frac{l}{3}) \\
&+ \frac{3}{8} l D_i \mathbf{b}(t + \frac{2}{3} l) + \frac{l}{48} E_i \mathbf{b}(t+l)) \quad i = 1, 2, 3, 4.
\end{aligned}
$$

Let

$$(I - \frac{1}{r_i} lA)^{-1} \mathbf{z}_i = \mathbf{y}_i, \quad i = 1,2,3,4$$

then

$$(I - \frac{1}{r_i} lA)\mathbf{y}_i = \mathbf{z}_i, \quad i = 1,2,3,4 \qquad (5.\ 38)$$

and

$$\mathbf{U}(t+l) = \mathbf{y}_1 + \mathbf{y}_2 + \mathbf{y}_3 + \mathbf{y}_4 \qquad (5.\ 39)$$

in which $\mathbf{y}_1$, $\mathbf{y}_2$, $\mathbf{y}_3$ and $\mathbf{y}_4$ are the solutions of the systems

$$(I - \frac{1}{r_i} \lambda lA)\mathbf{y}_i = \mathbf{z}_i, \quad i = 1,2,3,4 \qquad (5.\ 40)$$

respectively. This algorithm is presented in tabular form in Table 5.1.

5.3 Numerical Example

In this section a representative of many other methods based on (5.24) will only be used. Taking

$$a_1 = \frac{64}{25}$$

$$a_2 = \frac{7}{3}$$

and

$$a_3 = \frac{547}{600}$$

it is found that

$$r_1 = 2.1883713223893, \quad r_2 = 2.3398749224808$$

$$r_3 = 2.18837132239, \quad r_4 = 2.33987492248$$

are the real zeros of (5.69). These values produce

$$A_1 = -176.18490160503, \quad A_2 = 2051.1048759736,$$

$$A_3 = -1873.9199743685, \quad A_4 = 1873.9199743685,$$

$$B_1 = -176.18490160503, \quad B_2 = 2051.1048759736,$$

$$B_3 = -1873.9199743685, \quad B_4 = 1873.9199743685,$$

$$C_1 = -176.18490160503, \quad C_2 = 2051.1048759736,$$

$$C_3 = -1873.9199743685, \quad C_4 = 1873.9199743685,$$

$$D_1 = -176.18490160503, \quad D_2 = 2051.1048759736,$$

$$D_3 = -1873.9199743685, \quad D_4 = 1873.9199743685,$$

$$E_1 = -176.18490160503, \quad E_2 = 2051.1048759736,$$

$$E_3 = -1873.9199743685, \quad E_4 = 1873.9199743685$$

Consider once again the problem {(4.63)-(4.66)}, mentioned here for convenience,

$$\frac{\partial u}{\partial t} + 5\frac{\partial u}{\partial x} = \beta\frac{\partial^2 u}{\partial x^2}, \quad \beta > 0, \quad 0 < x < 1, \quad t > 0, \tag{5. 41}$$

subject to the boundary conditions

$$h_1(t) = u(0,t) = \sqrt{\frac{2}{2+\beta t}} \; exp\left(\frac{-(2+5t)^2}{4(2+\beta t)}\right), \quad t > 0, \tag{5. 42}$$

$$h_2(t) = u(1,t) = \sqrt{\frac{2}{2+\beta t}} \; exp\left(\frac{-(1+5t)^2}{4(2+\beta t)}\right), \quad t > 0, \tag{5. 43}$$

and the initial condition

$$g(x) = u(x,0) = exp\left(\frac{-(2-x)^2}{8}\right), \quad 0 \le x \le 1. \tag{5. 44}$$

This problem has theoretical solution

$$u(x,t) = \sqrt{\frac{2}{2+\beta t}} \; exp\left(\frac{-(x-5t-2)^2}{4(2+\beta t)}\right) \tag{5. 45}$$

(see Jain *et el.* [19]). Using the Algorithm developed in Section 5.2 with the information given at the beginning of this section the problem {(5.41)-(5.45)} is solved for $h = 0.1, 0.05, 0.025, 0.01, 0.005$ and $l = 0.1, 0.05, 0.025, 0.01, 0.005$ using $\beta = 1000$. In these experiments the method behaves smoothly with third-order accuracy over the whole interval $0 \leq x \leq 1$ and no contrived oscillations are observed. Maximum errors at time t=0.5 are observed at the mid-point of the region except for very small values of h and l and are given in Table 5.2. For $h = 0.05$ and $l = 0.001$ the maximum error and relative percentage error obtained are $-0.980D-14$ and $-0.157D-10$ respectively at point 8 of the discretization. It is noticed that the numerical solution crosses the analytical solution in this experiment but no oscillations are observed. The numerical solutions for $h = 0.1$ and $l = 0.1$ at time $t = 0.5$ is depicted in Figure 5.1.

Table 5.1: Algorithm 1

Steps	Processor 1	Processor 2	Processor 3	Processor 4
1 Input	$l, r_1, \mathbf{U}_0, A, A_1$ B_1, C_1, D_1, E_1	$l, r_2, \mathbf{U}_0, A, A_2$ B_2, C_2, D_2, E_2	$l, r_3, \mathbf{U}_0, A, A_3$ B_3, C_3, D_3, E_3	$l, r_4, \mathbf{U}_0, A, A_4$ B_4, C_4, D_4, E_4
2 Comp	$I - \frac{l}{r_1}A$	$I - \frac{l}{r_2}A$	$I - \frac{l}{r_3}A$	$I - \frac{l}{r_4}A$
3 Decom	$I - \frac{l}{r_1}A$ $= L_1U_1$	$I - \frac{l}{r_2}A$ $= L_2U_2$	$I - \frac{l}{r_3}A$ $= L_3U_3$	$I - \frac{l}{r_4}A$ $= L_4U_4$
4 Comp	$\mathbf{b}_1 = \mathbf{b}(t)$ $\mathbf{b}_2 = \mathbf{b}(t + \frac{l}{3})$ $\mathbf{b}_3 = \mathbf{b}(t + \frac{2l}{3})$ $\mathbf{b}_4 = \mathbf{b}(t + l)$	$\mathbf{b}_1 = \mathbf{b}(t)$ $\mathbf{b}_2 = \mathbf{b}(t + \frac{l}{3})$ $\mathbf{b}_3 = \mathbf{b}(t + \frac{2l}{3})$ $\mathbf{b}_4 = \mathbf{b}(t + l)$	$\mathbf{b}_1 = \mathbf{b}(t)$ $\mathbf{b}_2 = \mathbf{b}(t + \frac{l}{3})$ $\mathbf{b}_3 = \mathbf{b}(t + \frac{2l}{3})$ $\mathbf{b}_4 = \mathbf{b}(t + l)$	$\mathbf{b}_1 = \mathbf{b}(t)$ $\mathbf{b}_2 = \mathbf{b}(t + \frac{l}{3})$ $\mathbf{b}_3 = \mathbf{b}(t + \frac{2l}{3})$ $\mathbf{b}_4 = \mathbf{b}(t + l)$
5 Using	$\mathbf{w}_1(t)$ $= \frac{l}{48}\{2B_1\mathbf{b}_1$ $+9C_1\mathbf{b}_2$ $+18D_1\mathbf{b}_3$ $+E_1\mathbf{b}_4\}$	$\mathbf{w}_2(t)$ $= \frac{l}{48}\{2B_2\mathbf{b}_1$ $+9C_2\mathbf{b}_2$ $+18D_2\mathbf{b}_3$ $+E_2\mathbf{b}_4\}$	$\mathbf{w}_3(t)$ $= \frac{l}{48}\{2B_3\mathbf{b}_1$ $+9C_3\mathbf{b}_2$ $+18D_3\mathbf{b}_3$ $+E_3\mathbf{b}_4\}$	$\mathbf{w}_4(t)$ $= \frac{l}{48}\{2B_4\mathbf{b}_1$ $+9C_41\mathbf{b}_2$ $+18D_4\mathbf{b}_3$ $+E_4\mathbf{b}_4\}$
6 Solve	$L_1U_1\mathbf{y}_1(t)$ $= A_1\mathbf{U}(t)$ $+\mathbf{w}_1(t)$	$L_2U_2\mathbf{y}_2(t)$ $= A_2\mathbf{U}(t)$ $+\mathbf{w}_2(t)$	$L_3U_3\mathbf{y}_3(t)$ $= A_3\mathbf{U}(t)$ $+\mathbf{w}_3(t)$	$L_4U_4\mathbf{y}_4(t)$ $= A_4\mathbf{U}(t)$ $+\mathbf{w}_4(t)$
7	$\mathbf{U}(t + l) = \mathbf{y}_1(t) + \mathbf{y}_2(t) + \mathbf{y}_3(t) + \mathbf{y}_4(t)$			
8	GO TO Step 4 for next time step			

Table 5.2: Maximum errors for Example 1 at $t = 0.5$

h	0.1	0.05	0.025	0.01	0.005
N	9	19	39	99	199
$l = 0.1$	-0.107D-7 5	-0.107D-7 10	-0.107D-7 20	-0.107D-7 50	-0.107D-7 100
$l = 0.05$	-0.108D-8 5	-0.108D-8 10	-0.107D-8 20	-0.108D-8 50	-0.107D-8 100
$l = 0.025$	-0.119D-9 5	-0.119D-9 10	-0.119D-9 20	-0.117D-9 50	-0.115D-9 100
$l = 0.01$	-0.650D-11 5	-0.645D-11 10	-0.646D-11 20	-0.555D-11 51	-0.602D-11 107
$l = 0.005$	-0.660D-12 5	-0.615D-12 10	-0.669D-12 20	-0.515D-12 49	-0.709D-13 80

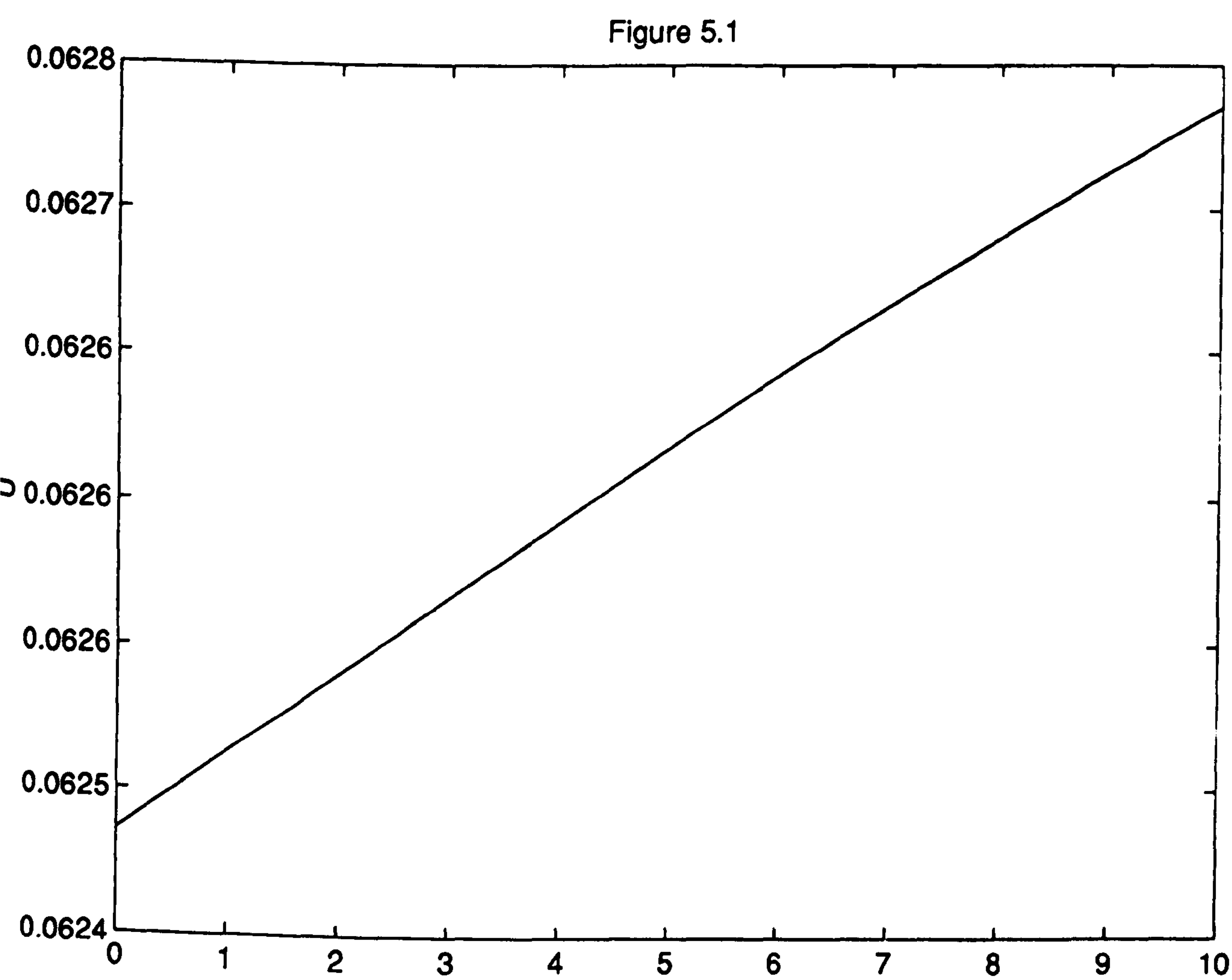

Figure 5.1: Numerical solution of example 1 for $h = 0.1$, and $l = 0.1$ at time t=0.5

Chapter 6

Third-Order Finite-Difference Methods for Second-Order Hyperbolic Partial Differential Equations

6.1 The Model Problem

Consider the one-dimensional initial/boundary-value ($IBVP$) problem consisting of the partial differential equation (PDE)

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}, \quad 0 < x < X, \ \ t > 0 \tag{6.1}$$

in which $u = u(x,t)$ subject to the homogeneous boundary conditions

$$u(0,t) = u(X,t) = 0, \quad t > 0 \tag{6.2}$$

and the initial conditions

$$u(x,0) = g(x), \quad 0 \le x \le X \tag{6.3}$$

$$\frac{\partial u(x,0)}{\partial t} = f(x), \quad 0 \le x \le X \tag{6.4}$$

in which $g(x)$ and $f(x)$ are given continuous functions of x.

There will exist discontinuities between the initial and the boundary conditions if

$$g(0) \neq 0 \quad \text{and/or} \quad g(X) \neq 0.$$

6.2 Discretization of $R \cup \partial R$

The region R (the open rectangle bounded by the lines $x = 0$, $t = 0$, $x = X$) and its boundary ∂R are covered by a grid, consisting of lines parallel to the time axis and lines parallel to the space axis (x-axis). Assuming $h > 0$ and $l > 0$, the interval $0 \leq x \leq X$ is divided into $N+1$ subintervals each of width h, so that

$$(N+1)h = X$$

and the time $t \geq 0$ is divided into equal time steps of length l. The parameter h is called the space-step and l is the time-step. Each discrete mesh point has co-ordinates of the form

$$(x_m, t_n) = (mh, nl)$$

for $m = 0, 1, 2, \ldots, N+1$ and $n = 0, 1, 2, \ldots$.

6.3 The Method

Replacing the space derivative $\frac{\partial^2 u(x,t)}{\partial x^2}$ in the PDE (6.1) by the third-order difference approximations [38]

$$\frac{\partial^2 u(x,t)}{\partial x^2} = \frac{1}{12h^2}\{11\,u(x-h,t) - 20\,u(x,t) + 6\,u(x+h,t)$$

$$+ \quad 4\,u(x+2h,t) - u(x+3h,t)\} + \frac{h^3}{12}\frac{\partial^5 u(x,t)}{\partial x^5}$$
$$+ \quad O(h^4)\, as \quad h \to 0 \qquad (6.\ 5)$$

for the mesh points (x_m, t_n) with $m = 1, 2, \ldots, N-2$,

$$\frac{\partial^2 u(x,t)}{\partial x^2} = \frac{1}{12h^2}\{u(x-3h,t) - 6\,u(x-2h,t) + 26\,u(x-h,t)$$
$$- \quad 40\,u(x,t) + 21\,u(x+h,t) - 2u(x+2h,t)\} + \frac{h^3}{12}\frac{\partial^5 u(x,t)}{\partial x^5}$$
$$+ \quad O(h^4)\, as \quad h \to 0 \qquad (6.\ 6)$$

for the mesh point (x_{N-1}, t_n) and

$$\frac{\partial^2 u(x,t)}{\partial x^2} = \frac{1}{12h^2}\{2\,u(x-4h,t) - 11\,u(x-3h,t) + 24\,u(x-2h,t)$$
$$- \quad 14\,u(x-h,t) - 10\,u(x,t) - 9\,u(x+h,t)\} + \frac{h^3}{12}\frac{\partial^5 u(x,t)}{\partial x^5}$$
$$+ \quad O(h^4)\, as \quad h \to 0 \qquad (6.\ 7)$$

for the mesh point (x_N, t_n), provides a system of N second-order ordinary differential equations $(ODE's)$ which can be written in matrix-vector form as

$$\frac{d^2\mathbf{U}(t)}{dt^2} = A\mathbf{U}(t), \quad t > 0 \qquad (6.\ 8)$$

with initial conditions

$$\mathbf{U}(0) = \mathbf{g} \qquad (6.\ 9)$$

and

$$\frac{d\mathbf{U}(0)}{dt} = \mathbf{f}(x) \qquad (6.\ 10)$$

in which

$$\begin{aligned}
\mathbf{U}(t) &= [U_1(t), U_2(t), \ldots, U_N(t)]^T, \\
\mathbf{g} &= [g(x_1), g(x_2), \ldots, g(x_N)]^T, \\
\mathbf{f} &= [f(x_1), f(x_2), \ldots, f(x_N)]^T,
\end{aligned}$$

T denoting transpose and

$$A = \frac{c^2}{12h^2}\begin{bmatrix} -20 & 6 & 4 & -1 & & & & & \bigcirc \\ 11 & -20 & 6 & 4 & -1 & & & & \\ & 11 & -20 & 6 & 4 & -1 & & & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & & \\ & & & 11 & -20 & 6 & 4 & -1 \\ & & & & 11 & -20 & 6 & 4 \\ & & & & 1 & -6 & 26 & -40 & 21 \\ \bigcirc & & & & 2 & -11 & 24 & -14 & -10 \end{bmatrix}_{N\times N} \quad (6.11)$$

It is noted that the approximations in (6.5), (6.6) and (6.7) all have the same leading error term $\frac{h^3}{12}\frac{\partial^5 u(x,t)}{\partial x^5}$, thus ensuring the same accuracy at all mesh points at time level t_n.

The eigenvalues of A are not known in closed form and must be calculated using, for instance, NAG subroutine F02AFF for a given vale of N. It will be seen that the stability of an algorithm can only be established if all eigenvalues of A, for a given N, have negative real parts.

The analytical solution of (6.8)–(6.10) is given by

$$\mathbf{U}(t) = \frac{1}{2}exp(tB)\{\mathbf{g} + B^{-1}\mathbf{f}\} + \frac{1}{2}exp(-tB)\{\mathbf{g} - B^{-1}\mathbf{f}\} \quad (6.12)$$

in which B is a square matrix of order N such that

$$B^2 = A.$$

For a time-step l, the semi-discrete solution $\mathbf{U}(t)$ satisfies the recurrence relation

$$\mathbf{U}(t+l) = \{exp(lB) + exp(-lB)\}\mathbf{U}(t) - \mathbf{U}(t-l), \quad t = l, 2l, \ldots. \quad (6.13)$$

Twizell [40].

6.4 Solution at the First Time-Step

Using Taylor's series

Substituting $t = l$ in (6.12) gives

$$\mathbf{U}(l) = \frac{1}{2}exp(lB)\{\mathbf{g} + B^{-1}\mathbf{f}\} + \frac{1}{2}exp(-lB)\{\mathbf{g} - B^{-1}\mathbf{f}\} \qquad (6.14)$$

which can be written as

$$\mathbf{U}(l) = \frac{1}{2}\left\{exp(lB) + exp(-lB)\right\}\mathbf{g} + \frac{1}{2}\left\{exp(lB) - exp(-lB)\right\}B^{-1}\mathbf{f}. \qquad (6.15)$$

Now

$$exp(lB) = I + lB + \frac{1}{2!}l^2B^2 + \frac{1}{3!}l^3B^3 + \frac{1}{4!}l^4B^4 + \frac{1}{5!}l^5B^5 + \frac{1}{6!}l^6B^6 + \frac{1}{7!}l^7B^7 + \dots \qquad (6.16)$$

and

$$exp(-lB) = I - lB + \frac{1}{2!}l^2B^2 - \frac{1}{3!}l^3B^3 + \frac{1}{4!}l^4B^4 - \frac{1}{5!}l^5B^5 + \frac{1}{6!}l^6B^6 - \frac{1}{7!}l^7B^7 + \dots \qquad (6.17)$$

Thus

$$exp(lB) + exp(-lB) = 2\left(I + \frac{1}{2!}l^2B^2 + \frac{1}{4!}l^4B^4 + \frac{1}{6!}l^6B^6 + \dots\right) \qquad (6.18)$$

and

$$exp(lB) - exp(-lB) = 2\left(lB + \frac{1}{3!}l^3B^3 + \frac{1}{5!}l^5B^5 + \frac{1}{7!}l^7B^7 + \dots\right) \qquad (6.19)$$

or

$$exp(lB) - exp(-lB) = 2\left\{I + \frac{1}{3!}l^2B^2 + \frac{1}{5!}l^4B^4 + \frac{1}{7!}l^6B^6 + \dots\right\} lB. \qquad (6.20)$$

Substituting these values in (6.15) gives

$$\begin{aligned} U(l) &= \left(I + \frac{1}{2!}l^2B^2 + \frac{1}{4!}l^4B^4 + \frac{1}{6!}l^6B^6 + \ldots\right)\mathbf{g} \\ &+ \left(I + \frac{1}{3!}l^2B^2 + \frac{1}{5!}l^4B^4 + \frac{1}{7!}l^6B^6 + \ldots\right)l\mathbf{f} \end{aligned} \quad (6.21)$$

or

$$U(l) = \left(I + \frac{1}{2!}l^2A + O(l^4)\right)\mathbf{g} + \left(I + \frac{1}{3!}l^2A + O(l^4)\right)l\mathbf{f}. \quad (6.22)$$

6.5 Rational Approximation to Matrix Exponential Function

To approximate the matrix exponential function in (6.13) consider the rational approximant (1.1)

$$E_3(\theta) = \frac{1 + (1-a_1)\theta + (\frac{1}{2} - a_1 + a_2)\theta^2}{1 - a_1\theta + a_2\theta^2 - (\frac{1}{6} - \frac{a_1}{2} + a_2)\theta^3}. \quad (6.23)$$

where a_1 and a_2 are parameters . Let

$$1 + (1-a_1)\theta + (\frac{1}{2} - a_1 + a_2)\theta^2 = p(\theta) \quad (6.24)$$

and

$$1 - a_1\theta + a_2\theta^2 - (\frac{1}{6} - \frac{a_1}{2} + a_2)\theta^3 = q(\theta). \quad (6.25)$$

Now consider the sum

$$E_3(\theta) + E_3(-\theta) = \frac{p(\theta)}{q(\theta)} + \frac{p(-\theta)}{q(-\theta)} = \frac{P(\theta)}{Q(\theta)} \quad (6.26)$$

where

$$\begin{aligned} P(\theta) &= p(\theta) \times q(-\theta) + p(-\theta) \times q(\theta) \\ &= 2\Big\{1 + (2a_2 - a_1^2 + \frac{1}{2})\theta^2 \\ &+ (\frac{3}{2}a_2 - 2a_1a_2 + a_2^2 - \frac{2}{3}a_1 + \frac{1}{2}a_1^2 + \frac{1}{6})\theta^4\Big\} \end{aligned} \quad (6.27)$$

and

$$
\begin{aligned}
Q(\theta) &= q(\theta) \times q(-\theta) \\
&= 1 + (2a_2 - a_1^2)\theta^2 - (\frac{1}{3}a_1 - a_1^2 + 2a_1a_2 - a_2^2)\theta^4 \\
&- (\frac{1}{6} + a_2 - \frac{1}{2}a_1)^2\theta^6. \qquad (6.28)
\end{aligned}
$$

Assuming $\phi = \theta^2$ gives

$$
\begin{aligned}
P(\phi) &= 2\Big\{1 + (2a_2 - a_1^2 + \frac{1}{2})\phi \\
&+ (\frac{3}{2}a_2 - 2a_1a_2 + a_2^2 - \frac{2}{3}a_1 + \frac{1}{2}a_1^2 + \frac{1}{6})\phi^2\Big\} \qquad (6.29)
\end{aligned}
$$

and

$$
\begin{aligned}
Q(\phi) &= 1 + (2a_2 - a_1^2)\phi - (\frac{1}{3}a_1 - a_1^2 + 2a_1a_2 - a_2^2)\phi^2 \\
&- (\frac{1}{6} + a_2 - \frac{1}{2}a_1)^2\phi^3. \qquad (6.30)
\end{aligned}
$$

6.6 Accuracy

It is convenient to consider the single initial-value problem

$$D^2y \equiv y''(t) = f(t,y), t > t_0, \quad y(t_0) = y_0, \quad y'(t_0) = z_0 \qquad (6.31)$$

where $y = y(t)$ and $D^2 = \frac{d^2}{dt^2}$. The numerical solution to this problem may be obtained from the formula

$$y(t+l) = \{exp(lD) + exp(-lD)\}y(t) - y(t-l). \qquad (6.32)$$

Replacing θ by lD in (6.26) and then substituting the value of $exp(lD) + exp(-lD)$ in (6.32) leads to

$$y_{n+1} = (a_1^2 - 2a_2)l^2y''_{n+1} + (\frac{a_1}{3} - a_1^2 + 2a_1a_2 - a_2^2)l^4y''''_{n+1}$$

$$
\begin{aligned}
&+ \quad (\frac{1}{6} - \frac{a_1}{2} + a_2)l^6 y_{n+1}^{''''''} + 2y_n + 2(\frac{1}{2} - a_1^2 + 2a_2)l^2 y_n^{''} \\
&+ \quad 2(\frac{1}{6} + \frac{3}{2}a_2 - 2a_1a_2 + a_2^2 - \frac{2}{3}a_1 + \frac{a_1^2}{2})l^4 y_n^{''''} - y_{n-1} \\
&- \quad (2a_2 - a_1^2)l^2 y_{n-1}^{''} - (\frac{a_1}{3} - a_1^2 + 2a_1a_2 - a_2^2)l^4 y_{n-1}^{''''} \\
&+ \quad (\frac{1}{6} - \frac{a_1}{2} + a_2)^2 l^6 y_{n-1}^{''''''} \qquad (6.33)
\end{aligned}
$$

in which y_n is an approximation to $y(t_n)$. The associated local truncation error is

$$
\begin{aligned}
L[y(t);l] &= y(t+l) - (a_1^2 - 2a_2)l^2 y^{''}(t+l) - (\frac{a_1}{3} - a_1^2 + 2a_1a_2 - a_2^2)l^4 y^{''''}(t+l) \\
&- (\frac{1}{6} - \frac{a_1}{2} + a_2)l^6 y^{''''''}(t+l) - 2y(t) - 2(\frac{1}{2} - a_1^2 + 2a_2)l^2 y^{''}(t) \\
&- 2(\frac{1}{6} + \frac{3}{2}a_2 - 2a_1a_2 + a_2^2 - \frac{2}{3}a_1 + \frac{a_1^2}{2})l^4 y^{''''}(t) + y(t-l) \\
&+ (2a_2 - a_1^2)l^2 y^{''}(t-l) - (\frac{a_1}{3} - a_1^2 + 2a_1a_2 - a_2^2)l^4 y^{''''}(t-l) \\
&- (\frac{1}{6} - \frac{a_1}{2} + a_2)^2 l^6 y^{''''''}(t-l) \qquad (6.34)
\end{aligned}
$$

which may be expanded as a Taylor series about t to give

$$
\begin{aligned}
L[y(t);l] &= y(t) + ly^{'}(t) + \frac{1}{2}l^2 y^{''}(t) + \frac{1}{6}l^3 y^{'''}(t) + \frac{1}{24}l^4 y^{''''}(t) + \frac{1}{120}l^5 y^{'''''}(t) \\
&\quad + \frac{1}{720}l^6 y^{''''''} + \ldots \\
&- (a_1^2 - 2a_2)l^2 \{y^{''}(t) + ly^{'''}(t) + \frac{1}{2}l^2 y^{''''}(t) + \frac{1}{6}l^3 y^{'''''}(t) + \frac{1}{24}l^4 y^{''''''} \\
&\quad + \ldots\} \\
&- (\frac{a_1}{3} - a_1^2 + 2a_1a_2 - a_2^2)l^4 \{y^{''''}(t) + ly^{'''''}(t) + \frac{1}{2}l^2 y^{''''''}(t) + \ldots\} \\
&- (\frac{1}{6} - \frac{a_1}{2} + a_2)^2 l^6 \{y^{''''''}(t) + \ldots\} \\
&- 2y(t) - 2(\frac{1}{2} - a_1^2 + 2a_2)l^2 y^{''}(t) \\
&- 2(\frac{1}{6} + \frac{3}{2}a_2 - 2a_1a_2 + a_2^2 - \frac{2}{3}a_1 + \frac{a_1^2}{2})l^4 y^{''''}(t) \\
&+ y(t) - ly^{'}(t) + \frac{1}{2}l^2 y^{''}(t) - \frac{1}{6}l^3 y^{'''}(t) + \frac{1}{24}l^4 y^{''''}(t) - \frac{1}{120}l^5 y^{'''''}(t)
\end{aligned}
$$

$$+\frac{1}{720}l^6y^{''''''}-\ldots$$

$$+\quad(2a_2-a_1^2)l^2\{y''(t)-ly'''(t)+\frac{1}{2}l^2y''''(t)-\frac{1}{6}l^3y'''''(t)+\frac{1}{24}l^4y''''''$$

$$-\ldots\}$$

$$-\quad(\frac{a_1}{3}-a_1^2+2a_1a_2-a_2^2)l^4\{y''''(t)-ly'''''(t)+\frac{1}{2}l^2y''''''(t)-\ldots\}$$

$$-\quad(\frac{1}{6}-\frac{a_1}{2}+a_2)^2l^6\{y''''''(t)-\ldots\}. \qquad (6.35)$$

After simplification (6.35) becomes

$$L[y(t);l]=(-\frac{1}{4}+\frac{1}{2}a_1-a_2)l^4y''''(t)+O(l^5). \qquad (6.36)$$

6.7 Development of Parallel Algorithm

Suppose that $r_i(i=1,2,3,r_i\neq 0)$ are distinct real zeros of $Q(\phi)$ defined by (6.30) then

$$exp(lB)+exp(-lB)=\sum_{i=1}^{3}c_i\left(I-\frac{l}{r_i}A\right)^{-1} \qquad (6.37)$$

where $B^2=A$ and c_i $(i=1,2,3)$, the partial-fraction coefficients, are defined by

$$c_i=\frac{P(r_i)}{\prod_{\substack{j=1\\ j\neq i}}^{3}\left(1-\frac{r_i}{r_j}\right)},\quad i=1,2,3 \qquad (6.38)$$

in which

$$\begin{aligned}P(r_i) &= 2\Big\{1+(2a_2-a_1^2+\frac{1}{2})r_i\\ &+ (\frac{3}{2}a_2-2a_1a_2+a_2^2-\frac{2}{3}a_1+\frac{1}{2}a_1^2+\frac{1}{6})r_i^2\Big\}\end{aligned}$$

$i=1,2,3$. So, using (6.31) in (6.13) gives

$$\mathbf{U}(t+l)=\left(\sum_{i=1}^{3}c_i\left(I-\frac{l^2}{r_i}A\right)^{-1}\right)\mathbf{U}(t)-\mathbf{U}(t-l). \qquad (6.39)$$

$t = l, 2l, 3l, \ldots$. Now let

$$c_i \left(I - \frac{l^2}{r_i} A \right)^{-1} \mathbf{U}(t) = \mathbf{w}_i(t), \quad i = 1, 2, 3, \qquad (6.40)$$

Then the systems of linear equations

$$\left(I - \frac{l^2}{r_i} A \right) \mathbf{w}_i(t) = c_i \mathbf{U}(t), \quad i = 1, 2, 3 \qquad (6.41)$$

can be solved for $\mathbf{w}_i(t) (i = 1, 2, 3)$ on three different processors simultaneously, and finally

$$\mathbf{U}(t + l) = \sum_{i=1}^{3} \mathbf{w}_i(t) - \mathbf{U}(t - l) \quad t = l, 2l, 3l, \ldots. \qquad (6.42)$$

This algorithm is given in tabular form in Table 6.1.

6.8 Numerical Examples

In this section a representative of many other methods based on (6.23) will only be used. So taking $a_1 = \frac{65431}{50000}$ and $a_2 = \frac{171151}{300000}$ as before gives

$r_1 = 4.7889690044658795$, $r_2 = 5.475014652818082$, $r_3 = 5.554994179738606$

as the real zeros of (6.30). Using these values in (6.38) gives

$c_1 = -352.369803216$, $c_2 = 4102.20974857$, $c_3 = -3747.83994535$

6.8.1 Example 1

Considering the one dimensional wave equation with constant coefficients (6.1) and taking $X = 1$, $g(x) = \frac{1}{8} sin(\pi x)$ and $f(x) = 0$ in {(6.1)-(6.4)} the model problem becomes

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}, \quad 0 < x < 1, \quad t > 0 \qquad (6.43)$$

subject to the initial conditions

$$u(x,0) = \frac{1}{8}sin(\pi x), \quad 0 \leq x \leq 1 \qquad (6.44)$$

$$\frac{\partial u(x,0)}{\partial t} = 0, \quad 0 \leq x \leq 1 \qquad (6.45)$$

and the boundary conditions

$$u(0,t) = u(1,t) = 0, \quad t > 0. \qquad (6.46)$$

This problem, which has theoretical solution

$$u(x,t) = \frac{1}{8}sin(\pi x) \ \ cos(c\pi t) \qquad (6.47)$$

has no discontinuities between the initial conditions and the boundary conditions at $x = 0$ and $x = 1$. The theoretical solution at time $t = 1.0$ is depicted in Figure 6.1.

Using the algorithm developed in Section 6.7 the model problem {(6.43)-(6.46)} is solved for h, l=0.1, 0.05, 0.025, 0.0125 using $c = \frac{1}{10}$ at time t=1.0, 2.0, and 3.0 In these experiments the method behaves smoothly over the whole interval $0 \leq x \leq 1$. The numerical solution for $h = 0.1$ and $l = 0.1$ at time t=1.0 is depicted in Figure 6.2. The profile depicted in Figure 6.2 (and in Figure 6.4 later) appears not to be smooth. This is because h and l are large and the software used (MATHEMATICA) joins the points associated with the calculations with straight lines. Comparing the peaks of Figure 6.1 and 6.2 confirms the accuracy of the method. The maximum absolute errors with positions are given in Table 6.2. It is clear from Table 6.2 that the method is third-order accurate for all values of t but error grows slightly as time increases.

6.8.2 Example 2

Considering the equation with constant coefficients (6.1) and taking $X = 0.5$, $g(x) = 0$) and $f(x) = sin(4\pi x)$ in {(6.1)-(6.4)} the model problem becomes

$$\frac{\partial^2 u}{\partial t^2} = \frac{1}{16\pi^2}\frac{\partial^2 u}{\partial x^2}, \quad 0 < x < 0.5, \quad t > 0 \qquad (6.48)$$

subject to the initial conditions

$$u(x,0) = 0, \quad 0 \le x \le 0.5 \qquad (6.49)$$

$$\frac{\partial u(x,0)}{\partial t} = sin(4\pi x), \quad 0 \le x \le 0.5 \qquad (6.50)$$

and the boundary conditions

$$u(0,t) = u(1,t) = 0, \quad t > 0. \qquad (6.51)$$

This problem, which has theoretical solution

$$u(x,t) = sin(4\pi x)\,sin(t) \qquad (6.52)$$

[6] has no discontinuities between the initial conditions and the boundary conditions at $x = 0$ and $x = 1$. The theoretical solution at time $t = 0.5$ is depicted in Figures 6.3.

The model problem {(6.48)-(6.51)} was also solved for h, l=0.05, 0.025, 0.0125, 0.00625 at time t=0.5 and 1.0. The method again behaves smoothly over the whole interval $0 \le x \le 0.5$ and gives maximum error at the centre of the region except for h, l=0.05 and 0.025. The numerical solution for $h = 0.05$ and $l = 0.05$ at time t=0.5 is depicted in Figure 6.4. Comparing the peaks and troughs of Figures 6.3 and 6.4 confirms the accuracy obtained using the method. All other numerical solutions produce better graphs. The maximum absolute errors with their positions are given in Table 6.3. It is clear from Table 6.3 that the method is third-order accurate for both values of t but maximum absolute error grows slightly as time increases.

Table 6.1: Algorithm 1

Steps	Processor 1	Processor 2	Processor 3
1 Input	$l, r_1, c_1,$ $\mathbf{U}_0, A$	$l, r_2, c_2,$ $\mathbf{U}_0, A$	$l, r_3, c_3,$ $\mathbf{U}_0, A$
2 Compute	$I - \frac{l}{r_1}A$	$I - \frac{l}{r_2}A$	$I - \frac{l}{r_3}A$
3 Decompose	$I - \frac{l}{r_1}A = L_1U_1$	$I - \frac{l}{r_2}A = L_2U_2$	$I - \frac{l}{r_3}A = L_3U_3$
4 Find	Solution at the first time step		
5 Solve	$L_1U_1\mathbf{w}_1(t) = c_1\mathbf{U}(t)$	$L_2U_2\mathbf{w}_2(t) = c_2\mathbf{U}(t)$	$L_3U_3\mathbf{w}_3(t) = c_3\mathbf{U}(t)$
6	$\mathbf{U}(t+l) = \mathbf{w}_1(t) + \mathbf{w}_2(t) + \mathbf{w}_3(t) - \mathbf{U}(t-l)$		
7	GO TO Step 5 for next time step		

Table 6.2: Maximum absolute errors for Example 1

N	9	19	39	79
h, l	0.1	0.05	0.025	0.0125
t=1.0 Positions	0.124847D-4 1	0.177997D-5 17	0.231373D-6 4	0.305657D-7 72
t=2.0 Positions	0.399566D-4 8	0.612910D-5 16	0.785875D-6 7	0.106804D-6 66
t=3.0 Positions	0.741103D-4 7	0.107269D-4 15	0.135521D-5 9	0.190258D-6 61

Positions are shown by space steps.

Table 6.3: Maximum absolute errors for Example 2

N	9	19	39	79
h, l	0.05	0.025	0.0125	0.00625
$t = 0.5$ Positions	0.386306D-3 4	0.512678D-4 9	0.650840D-5 20	0.818575D-6 40
$t = 1.0$ Positions	0.286251D-2 4	0.379984D-3 9	0.482384D-4 20	0.606705D-5 40

Positions are shown by space steps.

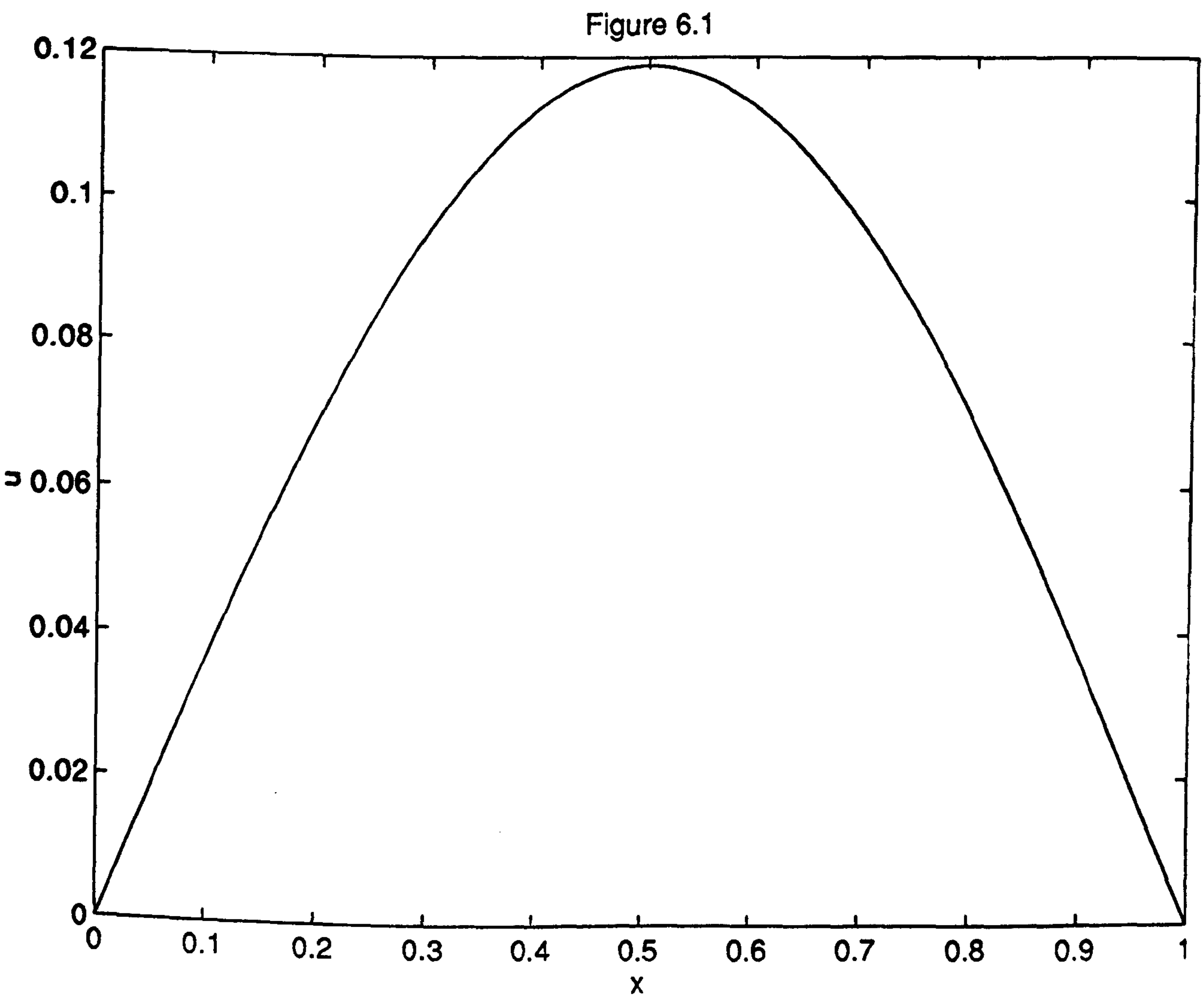

Figure 6.1: Theoretical solution of example 1 for time t=1.0

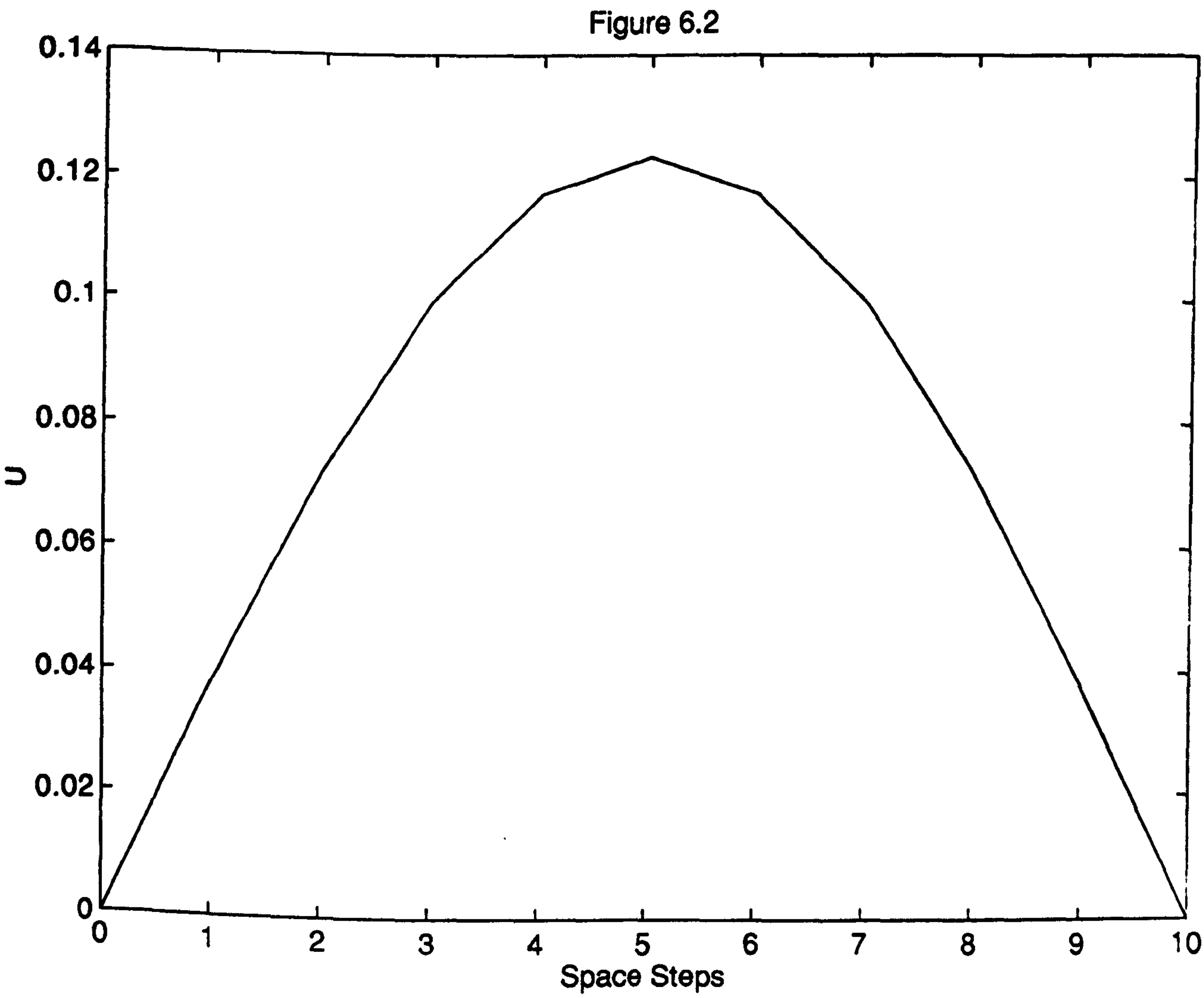

Figure 6.2: Numerical solution of example 1 for $h = 0.1$, and $l = 0.1$ at time t=1.0

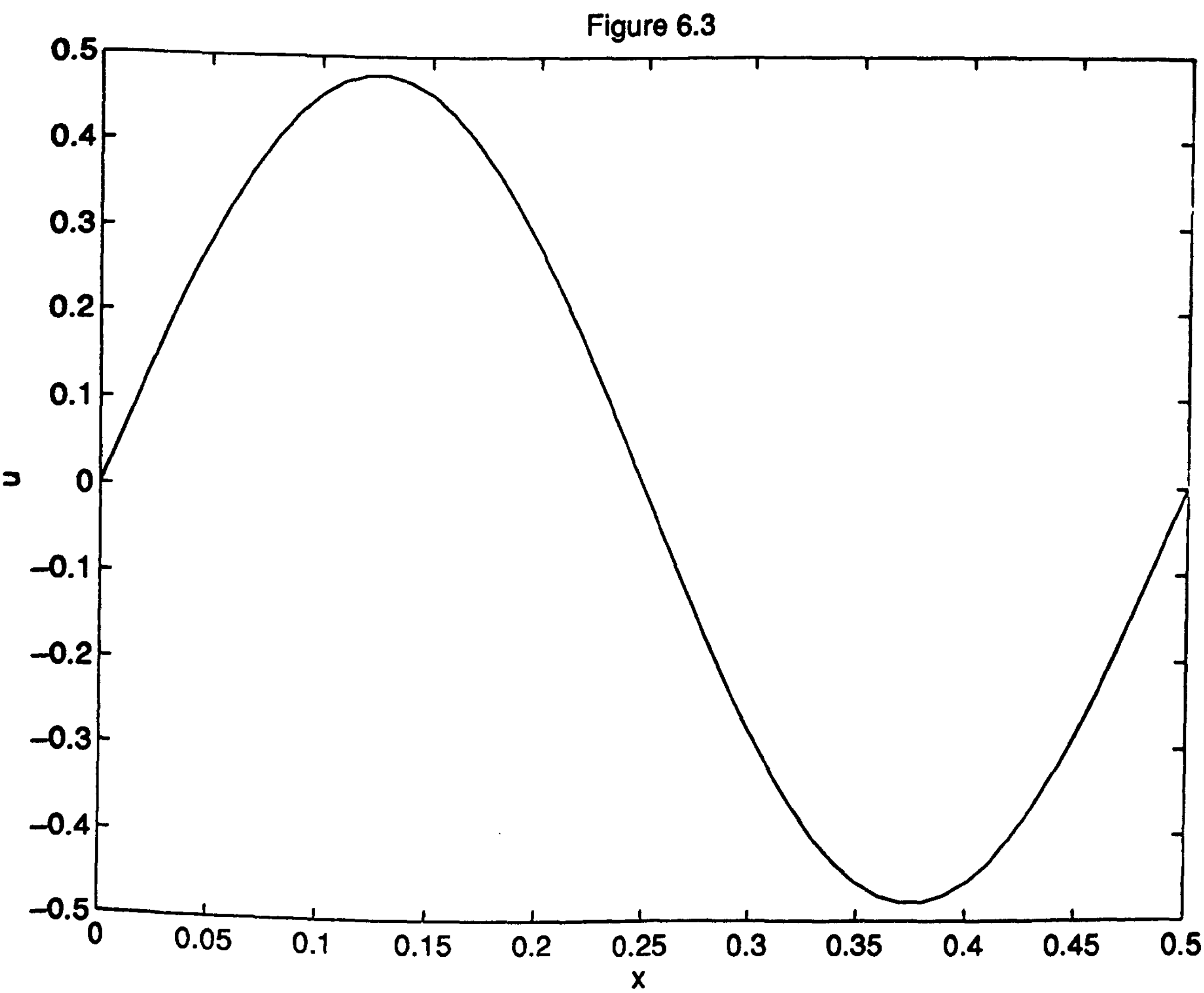

Figure 6.3: Theoretical solution of example 2 for time t=0.5

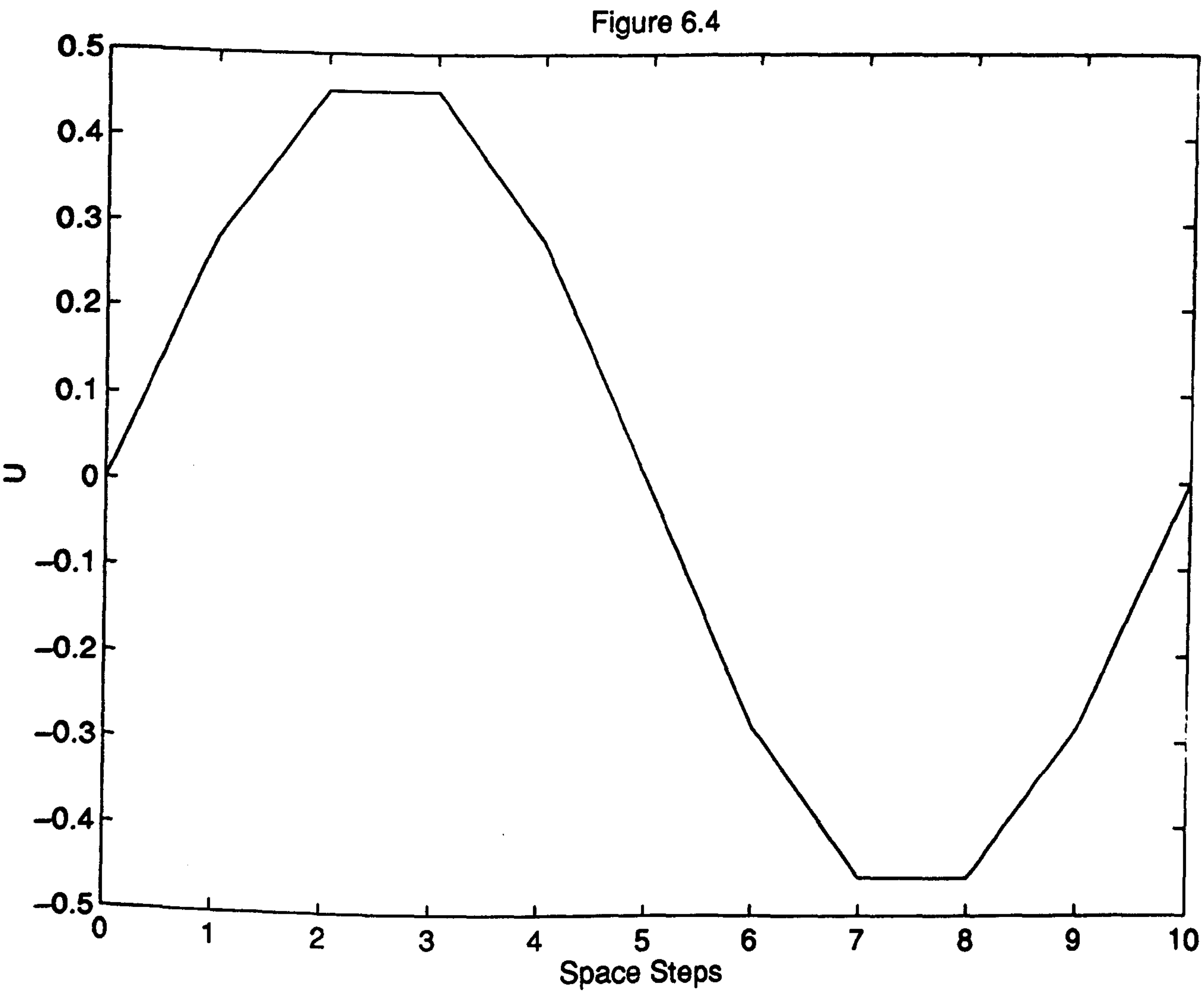

Figure 6.4: Numerical solution of example 2 for h, l=0.05 at time t=0.5

Chapter 7

Fourth-Order Finite-Difference Methods for Second-Order Hyperbolic Partial Differential Equations

---

7.1 The method

Considering the model problem of Chapter 6 consisting of the partial differential equation

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}, \quad 0 < x < X, \ \ t > 0 \tag{7. 1}$$

in which $u = u(x, t)$ subject to the boundary conditions

$$u(0, t) = u(X, t) = 0, \quad t > 0 \tag{7. 2}$$

and the initial conditions

$$u(x, 0) = g(x), \quad 0 \leq x \leq X \tag{7. 3}$$

$$\frac{\partial u(x, 0)}{\partial t} = f(x), \quad 0 \leq x \leq X, \tag{7. 4}$$

in which $g(x)$ and $f(x)$ are given continuous functions of x, the method can be developed by replacing the space derivative $\frac{\partial^2 u(x,t)}{\partial x^2}$ in (7.1) by the fourth-order difference approximations [39]

$$\begin{aligned}\frac{\partial^2 u(x,t)}{\partial x^2} &\simeq \frac{1}{12h^2}\{9u(x-h,t)-9u(x,t)-19u(x+h,t)\\ &+ 34u(x+2h,t)-21u(x+3h,t)+7u(x+4h,t)\\ &- u(x+5h,t)\}+\frac{h^4}{90}\frac{\partial^6 u(x,t)}{\partial x^6}\\ &+ O(h^5)\,as\;\; h\to 0 \end{aligned} \qquad (7.5)$$

for the mesh point (x_1, t_n),

$$\begin{aligned}\frac{\partial^2 u(x,t)}{\partial x^2} &\simeq \frac{1}{12h^2}\{-u(x-2h,t)+16u(x-h,t)-30u(x,t)\\ &+ 16u(x+h,t)-u(x+2h,t)\}+\frac{h^4}{90}\frac{\partial^6 u(x,t)}{\partial x^6}\\ &+ O(h^5)\,as\;\; h\to 0 \end{aligned} \qquad (7.6)$$

for the mesh points (x_m, t_n) with $m = 2, 3, \ldots, N-1$ and

$$\begin{aligned}\frac{\partial^2 u(x,t)}{\partial x^2} &\simeq \frac{1}{12h^2}\{-u(x-5h,t)+7u(x-4h,t)-21\,u(x-3h,t)\\ &+ 34u(x-2h,t)-19u(x-h,t)-9u(x,t)+9u(x+h,t)\}\\ &+ \frac{h^4}{90}\frac{\partial^6 u(x,t)}{\partial x^6}+O(h^5)\,as\;\; h\to 0 \end{aligned} \qquad (7.7)$$

for the mesh point (x_N, t_n), provides a system of N second-order ordinary differential equations which can be written in vector-matrix form as

$$\frac{d^2\mathbf{U}(t)}{dt^2} = A\mathbf{U}(t), \quad t > 0 \qquad (7.8)$$

with initial conditions

$$\mathbf{U}(0) = \mathbf{g} \qquad (7.9)$$

and

$$\frac{d\mathbf{U}(0)}{dt} = \mathbf{f}(x) \qquad (7.10)$$

in which

$$\begin{aligned}\mathbf{U}(t) &= [U_1(t), U_2(t), \ldots, U_N(t)]^T,\\ \mathbf{g} &= [g(x_1), g(x_2), \ldots, g(x_N)]^T,\\ \mathbf{f} &= [f(x_1), f(x_2), \ldots, f(x_N)]^T,\end{aligned}$$

T denoting transpose and

$$A = \frac{c^2}{12h^2}\begin{bmatrix} -9 & -19 & 34 & -21 & 7 & -1 & & & \bigcirc \\ 16 & -30 & 16 & -1 & & & & & \\ -1 & 16 & -30 & 16 & -1 & & & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & & & \\ & & -1 & 16 & -30 & 16 & -1 & & \\ & & & -1 & 16 & -30 & 16 & -1 & \\ & & & & -1 & 16 & -30 & 16 & \\ \bigcirc & & -1 & 7 & -21 & 34 & -19 & -9 & \end{bmatrix}_{N\times N} \qquad (7.11)$$

It is noted that the approximations in (7.5), (7.6) and (7.7) all have the same leading error term $\frac{h^4}{90}\frac{\partial^6 u(x,t)}{\partial x^6}$, thus ensuring the same accuracy at all mesh points at time level t_n.

The eigenvalues of A must have negative real parts to ensure the stability of the algorithm to be developed. These eigenvalues are not known in closed form and must be calculated for a given value of N using software such as NAG subroutine F02AFF.

7.2 Solution at the First Time-Step

Using Taylor's series

Substituting $t = l$ in (6.12) gives

$$\mathbf{U}(l) = \frac{1}{2}exp(lB)\{\mathbf{g} + B^{-1}\mathbf{f}\} + \frac{1}{2}exp(-lB)\{\mathbf{g} - B^{-1}\mathbf{f}\} \qquad (7.12)$$

which can be written as

$$\mathbf{U}(l) = \frac{1}{2}\{exp(lB) + exp(-lB)\}\,\mathbf{g} + \frac{1}{2}\{exp(lB) - exp(-lB)\}\,B^{-1}\mathbf{f}. \qquad (7.13)$$

Now

$$exp(lB) = I + lB + \frac{1}{2!}l^2B^2 + \frac{1}{3!}l^3B^3 + \frac{1}{4!}l^4B^4 + \frac{1}{5!}l^5B^5 + \frac{1}{6!}l^6B^6 + \frac{1}{7!}l^7B^7 + \dots \tag{7. 14}$$

and

$$exp(-lB) = I - lB + \frac{1}{2!}l^2B^2 - \frac{1}{3!}l^3B^3 + \frac{1}{4!}l^4B^4 - \frac{1}{5!}l^5B^5 + \frac{1}{6!}l^6B^6 - \frac{1}{7!}l^7B^7 + \dots \tag{7. 15}$$

Thus

$$exp(lB) + exp(-lB) = 2\left(I + \frac{1}{2!}l^2B^2 + \frac{1}{4!}l^4B^4 + \frac{1}{6!}l^6B^6 + \dots\right) \tag{7. 16}$$

and

$$exp(lB) - exp(-lB) = 2\left(lB + \frac{1}{3!}l^3B^3 + \frac{1}{5!}l^5B^5 + \frac{1}{7!}l^7B^7 + \dots\right) \tag{7. 17}$$

or

$$exp(lB) - exp(-lB) = 2\left\{I + \frac{1}{3!}l^2B^2 + \frac{1}{5!}l^4B^4 + \frac{1}{7!}l^6B^6 + \dots\right\} lB \tag{7. 18}$$

Substituting these values in (7.13) gives

$$\begin{aligned} \mathbf{U}(l) &= \left(I + \frac{1}{2!}l^2B^2 + \frac{1}{4!}l^4B^4 + \frac{1}{6!}l^6B^6 + \dots\right)\mathbf{g} \\ &+ \left(I + \frac{1}{3!}l^2B^2 + \frac{1}{5!}l^4B^4 + \frac{1}{7!}l^6B^6 + \dots\right)l\mathbf{f} \end{aligned} \tag{7. 19}$$

or

$$\begin{aligned} \mathbf{U}(l) &= \left(I + \frac{1}{2!}l^2A + \frac{1}{4!}l^4A^2 + O(l^5)\right)\mathbf{g} \\ &+ \left(I + \frac{1}{3!}l^2A + O(l^5)\right)l\mathbf{f}. \end{aligned} \tag{7. 20}$$

7.3 Rational Approximation to Matrix Exponentional Function

To approximate the matrix exponential functions in (7.13) consider the rational approximant (1.2), given for a real scalar θ, by

$$E_4(\theta) = \frac{1+(1-a_1)\theta+(\frac{1}{2}-a_1+a_2)\theta^2+(\frac{1}{6}-\frac{1}{2}a_1+a_2-a_3)\theta^3}{1-a_1\theta+a_2\theta^2-a_3\theta^3+(-\frac{1}{24}+\frac{a_1}{6}-\frac{a_2}{2}+a_3)\theta^4}. \quad (7.21)$$

where a_1 a_2 and a_3 are parameters . Let

$$1+(1-a_1)\theta+(\frac{1}{2}-a_1+a_2)\theta^2+(\frac{1}{6}-\frac{a_1}{2}+a_2-a_3)\theta^3 = p(\theta) \quad (7.22)$$

and

$$1-a_1\theta+a_2\theta^2-a_3\theta^3+(-\frac{1}{24}+\frac{a_1}{6}-\frac{a_2}{2}+a_3)\theta^4 = q(\theta). \quad (7.23)$$

Now consider the sum

$$E_4(\theta)+E_4(-\theta) = \frac{p(\theta)}{q(\theta)}+\frac{p(-\theta)}{q(-\theta)} = \frac{P(\theta)}{Q(\theta)} \quad (7.24)$$

where

$$\begin{aligned} P(\theta) &= p(\theta)\times q(-\theta)+p(-\theta)\times q(\theta) \\ &= 2\Big\{1+(2a_2-a_1^2+\frac{1}{2})\theta^2+(\frac{1}{3}a_1-\frac{1}{2}a_1^2-2a_1a_3+2a_3+a_2^2-\frac{1}{24})\theta^4 \\ &+ (\frac{a_3}{6}-\frac{3}{2}a_1a_3+2a_2a_3+\frac{a_1}{8}-\frac{7}{24}a_2-\frac{a_1^2}{6}+\frac{2}{3}a_1a_2-\frac{a_2^2}{2}-\frac{1}{48})\theta^6\Big\} \end{aligned} \quad (7.25)$$

and

$$\begin{aligned} Q(\theta) &= q(\theta)\times q(-\theta) \\ &= 1+(2a_2-a_1^2)\theta^2+(\frac{1}{3}a_1-a_2+2a_3-2a_1a_3+a_2^2-\frac{1}{12})\theta^4 \\ &+ (\frac{1}{3}a_1a_2+2a_2a_3-a_2^2-\frac{a_2}{12}-a_3^2)\theta^6 \\ &+ (-\frac{1}{24}+\frac{a_1}{6}-\frac{a_2}{2}+a_3)^2\theta^8. \end{aligned} \quad (7.26)$$

Assuming $\phi = \theta^2$ gives

$$\begin{aligned} P(\phi) &= 2\Big\{1 + (2a_2 - a_1^2 + \frac{1}{2})\phi + (\frac{1}{3}a_1 - \frac{1}{2}a_1^2 - 2a_1a_3 + 2a_3 + a_2^2 - \frac{1}{24})\phi^2 \\ &+ (\frac{a_3}{6} - \frac{3}{2}a_1a_3 + 2a_2a_3 + \frac{a_1}{8} - \frac{7}{24}a_2 - \frac{a_1^2}{6} + \frac{2}{3}a_1a_2 - \frac{a_2^2}{2} - \frac{1}{48})\phi^3\Big\} \end{aligned} \quad (7.27)$$

and

$$\begin{aligned} Q(\phi) &= 1 + (2a_2 - a_1^2)\phi + (\frac{1}{3}a_1 - a_2 + 2a_3 - 2a_1a_3 + a_2^2 - \frac{1}{12})\phi^2 \\ &+ (\frac{1}{3}a_1a_2 + 2a_2a_3 - a_2^2 - \frac{a_2}{12} - a_3^2)\phi^3 \\ &+ (-\frac{1}{24} + \frac{a_1}{6} - \frac{a_2}{2} + a_3)^2\phi^4. \end{aligned} \quad (7.28)$$

7.4 Accuracy

It is convenient to consider the single initial-value problem as in Chapter 6

$$D^2y \equiv y''(t) = f(t,y). \ \ t > t_0, \ \ y(t_0) = y_0, \ \ y'(t_0) = z_0, \quad (7.29)$$

where $y = y(t)$ and $D^2 \equiv \frac{d^2}{dt^2}$. The numerical solution to this problem may be obtained from the formula

$$y(t+l) = \{exp(lD) + exp(-lD)\}y(t) - y(t-l). \quad (7.30)$$

Replacing θ by lD in (7.24) and then substituting the value of $exp(lD) + exp(-lD)$ in (7.30) leads to

$$\begin{aligned} y(t+l) &= -\{q_1l^2y''(t+l) + q_2l^4y^{(4)}(t+l) + q_3l^6y^{(6)}(t+l) + q_4l^8y^{(8)}(t+l)\} \\ &+ 2\{y(t) + p_1l^2y''(t) + p_2l^4y^{(4)}(t) + p_3l^6y^{(6)}(t)\} \\ &- \{y(t-l) + q_1l^2y''(t-l) + q_2l^4y^{(4)}(t-l) + q_3l^6y^{(6)}(t-l) \\ &\quad + q_4l^8y^{(8)}(t-l)\} \end{aligned} \quad (7.31)$$

in which y_n is an approximation to $y(t_n)$ and

$$
\begin{aligned}
p_1 = & \quad 2a_2 - a_1^2 + \tfrac{1}{2}, \\
p_2 = & \quad \tfrac{a_1}{3} - \tfrac{a_1^2}{2} - 2a_1a_3 + 2a_3 + a_2^2 - \tfrac{1}{24}, \\
p_3 = & \quad \{\tfrac{a_3}{6} - \tfrac{3}{2}a_1a_3 + 2a_2a_3 + \tfrac{a_1}{8} \\
& \quad -\tfrac{7}{24}a_2 - \tfrac{a_1^2}{6} + \tfrac{2}{3}a_1a_2 - \tfrac{a_2^2}{2} - \tfrac{1}{48}\}, \\
q_1 = & \quad 2a_2 - a_1^2, \\
q_2 = & \quad \tfrac{a_1}{3} - a_2 - 2a_1a_3 + 2a_3 + a_2^2 - \tfrac{1}{12}, \\
q_3 = & \quad \tfrac{1}{3}a_1a_2 - \tfrac{a_2}{12} + 2a_2a_3 - a_2^2 - a_3^2, \\
q_4 = & \quad (-\tfrac{1}{24} + \tfrac{a_1}{6} - \tfrac{a_2}{2} + a_3)^2.
\end{aligned}
$$

The associated local truncation error is

$$
\begin{aligned}
L[y(t);l] \quad = & \quad y(t+l) + q_1 l^2 y''(t+l) + q_2 l^4 y^{(4)}(t+l) + q_3 l^6 y^{(6)}(t+l) \\
& \quad + q_4 l^8 y^{(8)}(t+l) \\
- & \quad 2\{y(t) + p_1 l^2 y''(t) + p_2 l^4 y^{(4)}(t) + p_3 l^6 y^{(6)}(t)\} \\
+ & \quad \{y(t-l) + q_1 l^2 y''(t-l) + q_2 l^4 y^{(4)}(t-l) + q_3 l^6 y^{(6)}(t-l) \\
& \quad + q_4 l^8 y^{(8)}(t-l)\} \qquad (7.\ 32)
\end{aligned}
$$

or

$$
\begin{aligned}
L[y(t);l] \quad = & \quad y(t+l) + y(t-l) \\
+ & \quad q_1 l^2 \{y''(t+l) + y''(t-l)\} \\
+ & \quad q_2 l^4 \{y^{(4)}(t+l) + y^{(4)}(t-l)\} \\
+ & \quad q_3 l^6 \{y^{(6)}(t+l) + y^{(6)}(t-l)\} \\
+ & \quad q_4 l^8 \{y^{(8)}(t+l) + y^{(8)}(t-l)\} \\
- & \quad 2\{y(t) + p_1 l^2 y''(t) + p_2 l^4 y^{(4)}(t) + p_3 l^6 y^{(6)}(t)\} \qquad (7.\ 33)
\end{aligned}
$$

which may be expanded as a Taylor series about $y(t)$ to give

$$
\begin{aligned}
L[y(t);l] \quad = & \quad 2\{y(t) + \frac{l^2}{2}y'' + \frac{l^4}{24}y^{(4)} + \frac{l^6}{720}y^{(6)} + \ldots\} \\
+ & \quad 2q_1 l^2 \{y''(t) + \frac{l^2}{2}y^{(4)} + \frac{l^4}{24}y^{(6)} + \frac{l^6}{720}y^{(8)} + \ldots\} \\
+ & \quad 2q_2 l^4 \{y^{(4)}(t) + \frac{l^2}{2}y^{(6)} + \frac{l^4}{24}y^{(8)} + \frac{l^6}{720}y^{(10)} + \ldots\}
\end{aligned}
$$

$$
\begin{aligned}
&+ \quad 2q_3 l^6\{y^{(6)}(t) + \frac{l^2}{2}y^{(8)} + \frac{l^4}{24}y^{(10)} + \ldots\} \\
&+ \quad 2q_4 l^8\{y^{(8)}(t) + \frac{l^2}{2}y^{(10)} + \ldots\} \\
&- \quad 2\{y(t) + p_1 l^2 y''(t) + p_2 l^4 y^{(4)}(t) + p_3 l^6 y^{(6)}(t)\} \qquad (7.34)
\end{aligned}
$$

After simplification (7.34) becomes

$$
\begin{aligned}
L[y(t);l] &= (1 + 2q_1 - 2p_1)l^2 y''(t) \\
&+ (\frac{1}{12} + q_1 + 2q_2 - 2p_2)l^4 y^{(4)}(t) \\
&+ (\frac{1}{360} + \frac{q_1}{12} + q_2 + 2q_3 - 2p_3)l^6 y^{(6)}(t) \\
&+ O(l^8). \qquad (7.35)
\end{aligned}
$$

Using the values of p_i and q_i $(i = 1, 2, 3)$ in (7.35) gives

$$
\begin{aligned}
L[y(t);l] &= \{-\frac{149}{360} + \frac{5}{3}a_1 - 4a_2 + 2a_3 - \frac{13}{12}a_1^2 - 3a_2^2 - a_3^2 \\
&+ \frac{14}{3}a_1 a_2 - 2a_1 a_3 + 4a_2 a_3\}l^6 y^{(6)}(t) + O(l^8). \qquad (7.36)
\end{aligned}
$$

7.5 Development of Parallel Algorithm

Suppose that $r_i (i = 1, 2, 3, 4, r_i \neq 0)$ are the distinct real zeros of $Q(\phi)$ defined by (7.28) then

$$
exp(lB) + exp(-lB) = \sum_{i=1}^{4} c_i \left(I - \frac{l}{r_i}A\right)^{-1} \qquad (7.37)
$$

where $B^2 = A$ and c_i $(i = 1, 2, 3, 4)$, the partial-fraction coefficients, are defined by

$$
c_i = \frac{P(r_i)}{\prod_{\substack{j=1 \\ j \neq i}}^{4} \left(1 - \frac{r_i}{r_j}\right)}, \quad i = 1, 2, 3, 4 \qquad (7.38)
$$

in which

$$P(r_i) = 2\Big\{1 + (2a_2 - a_1^2 + \frac{1}{2})r_i + (\frac{1}{3}a_1 - \frac{1}{2}a_1^2 - 2a_1a_3 + 2a_3 + a_2^2 - \frac{1}{24})r_i^2$$
$$+ (\frac{a_3}{6} - \frac{3}{2}a_1a_3 + 2a_2a_3 + \frac{a_1}{8} - \frac{7}{24}a_2 - \frac{a_1^2}{6} + \frac{2}{3}a_1a_2 - \frac{a_2^2}{2} - \frac{1}{48})r_i^3\Big\} \quad (7.39)$$

$i = 1, 2, 3, 4$. So, using (7.37) in (6.13) gives

$$\mathbf{U}(t+l) = \left(\sum_{i=1}^{4} c_i \left(I - \frac{l^2}{r_i}A\right)^{-1}\right)\mathbf{U}(t) - \mathbf{U}(t-l), \quad (7.40)$$

$t = l, 2l, 3l, \ldots$. Now let

$$c_i \left(I - \frac{l^2}{r_i}A\right)^{-1} \mathbf{U}(t) = \mathbf{w}_i(t), \quad i = 1, 2, 3, 4 \quad (7.41)$$

Then the systems of linear equations

$$\left(I - \frac{l^2}{r_i}A\right)\mathbf{w}_i(t) = c_i\mathbf{U}(t), \quad i = 1, 2, 3, 4 \quad (7.42)$$

can be solved for $\mathbf{w}_i(t)(i = 1, 2, 3, 4)$ on four different processors simultaneously, and finally

$$\mathbf{U}(t+l) = \sum_{i=1}^{4} \mathbf{w}_i(t) - \mathbf{U}(t-l) \quad t = l, 2l, 3l, \ldots. \quad (7.43)$$

This algorithm is given in tabular form in Table 7.1.

7.6 Numerical Examples

As in Chapter 6, a representative of methods based on (7.21) will be used. So, taking $c = 0.1$, $a_1 = \frac{64}{25}$, $a_2 = \frac{7}{3}$ and $a_3 = \frac{547}{600}$ as before gives

$$r_1 = 0.879057959205939, \quad r_2 = 3.293208163041111,$$

$$r_3 = 4.000000000000405, \quad r_4 = 5.109949525352754$$

as the real zeros of (7.28). Using these values in (7.38) gives

$$c_1 = -0.243656912725722D+03, \quad c_2 = 0.506244897959209D+03,$$

$$c_3 = -0.262087555440892D+03, \quad c_4 = 0.149957020740562D+01$$

7.6.1 Example 1

Considering the one dimensional problem {(7.1)-(7.4)} with $X = 1$, $g(x) = \frac{1}{8}sin(\pi x)$ and $f(x) = 0$ the model problem becomes

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}, \qquad 0 < x < 1, \quad t > 0 \qquad (7.44)$$

subject to the initial conditions

$$u(x,0) = \frac{1}{8}sin(\pi x), \quad 0 \le x \le 1, \qquad (7.45)$$

$$\frac{\partial u(x,0)}{\partial t} = 0, \qquad 0 \le x \le 1, \qquad (7.46)$$

and the boundary conditions

$$u(0,t) = u(1,t) = 0, \quad t > 0. \qquad (7.47)$$

This problem has theoretical solution

$$u(x,t) = \frac{1}{8}sin(\pi x)cos(c\pi t). \qquad (7.48)$$

The theoretical solution at time $t = 1.0$ is depicted in Figure 6.1.

Using Algorithm 1 the model problem {(7.44)-(7.47)} is solved for $l, h = \frac{1}{12}, \frac{1}{24}, \frac{1}{48}, \frac{1}{96}$, using $c = \frac{1}{10}$ at t=1.0, 2.0 and 3.0. In these experiments the method behaves smoothly over the whole interval $0 \le x \le 1$ and gives maximum error at the centre of the region except for $h = \frac{1}{12}$. The numerical solution for $h, l = \frac{1}{12}$ at time t=1.0 is depicted in Figure 7.1. All other numerical solutions produce similar graphs. Maximum absolute errors with positions are given in Table 7.2. It is clear from Table 7.2 that the new method is better than fourth order for larger values of h and l and it is fourth-order over all. Table 7.2 shows that with the passage of time the maximum absolute error grows slightly.

7.6.2 Example 2

Considering the one dimensional hyperbolic problem

$$\frac{\partial^2 u}{\partial t^2} = \frac{1}{16\pi^2}\frac{\partial^2 u}{\partial x^2}, \quad 0 < x < 0.5, \quad t > 0 \qquad (7.49)$$

subject to the initial conditions

$$u(x,0) = 0, \quad 0 \le x \le 0.5 \qquad (7.50)$$

$$\frac{\partial u(x,0)}{\partial t} = sin(4\pi x), \quad 0 \le x \le 0.5 \qquad (7.51)$$

and the boundary conditions

$$u(0,t) = u(1,t) = 0, \quad t > 0. \qquad (7.52)$$

The theoretical solution of this problem

$$u(x,t) = sin(4\pi x)\, sin(t) \qquad (7.53)$$

([6]) at time $t = 0.5$ is depicted in Figure 6.3.

Using again Algorithm 1 the model problem {(7.49)-(7.52)} is solved for $l, h = \frac{1}{24}, \frac{1}{48}, \frac{1}{96}, \frac{1}{192}$ at t=0.5 and 1.0. In these experiments the method behaves smoothly over the whole interval $0 \le x \le 0.5$. The numerical solution for $h, l = \frac{1}{24}$ at time t=0.5 is depicted in Figure 7.2. All other numerical solutions produce better graphs. Maximum absolute errors with positions are given in Table 7.3. It is clear from Table 7.3 that the method is fourth order but with the passage of time maximum absolute error grows slightly.

Table 7.1: Algorithm 1

Steps	Processor 1	Processor 2	Processor 3	Processor 4
1 Input	l, r_1, c_1, $\mathbf{U}_0, A$	l, r_2, c_2, $\mathbf{U}_0, A$	l, r_3, c_3, $\mathbf{U}_0, A$	l, r_4, c_4, $\mathbf{U}_0, A$
2 Compute	$I - \frac{l}{r_1}A$	$I - \frac{l}{r_2}A$	$I - \frac{l}{r_3}A$	$I - \frac{l}{r_4}A$
3 Decompose	$I - \frac{l}{r_1}A = L_1U_1$	$I - \frac{l}{r_2}A = L_2U_2$	$I - \frac{l}{r_3}A = L_3U_3$	$I - \frac{l}{r_4}A = L_4U_4$
4 Find	Solution at the first time step			
5 Solve	$L_1U_1\mathbf{w}_1(t) = c_1\mathbf{U}(t)$	$L_2U_2\mathbf{w}_2(t) = c_2\mathbf{U}(t)$	$L_3U_3\mathbf{w}_3(t) = c_3\mathbf{U}(t)$	$L_4U_4\mathbf{w}_4(t) = c_4\mathbf{U}(t)$
6	$\mathbf{U}(t+l) = \mathbf{w}_1(t) + \mathbf{w}_2(t) + \mathbf{w}_3(t) + \mathbf{w}_4(t) - \mathbf{U}(t-l)$			
7	GO TO Step 5 for next time step			

Table 7.2: Maximum absolute errors for Example 1.

N	11	23	47	95
h, l	$\frac{1}{12}$	$\frac{1}{24}$	$\frac{1}{48}$	$\frac{1}{96}$
t=1.0 Positions	0.52028D-6 1,11	0.19602D-7 12	0.12301D-8 24	0.92815D-10 50
t=2.0 Positions	0.13930D-5 1,11	0.74557D-7 12	0.46802D-8 24	0.35069D-9 48
t=3.0 Positions	0.24834D-5 3,9	0.15392D-6 12	0.96614D-8 24	0.72430D-9 48

Positions are shown by space steps.

Table 7.3: Maximum absolute errors for Example 2.

N	11	23	47	95
h, l	$\frac{1}{24}$	$\frac{1}{48}$	$\frac{1}{96}$	$\frac{1}{192}$
$t = 0.5$ Positions	0.23782D-4 1,11	0.16556D-5 1,23	0.65911D-7 12,36	0.41566D-8 72
$t = 1.0$ Positions	0.16556D-3 1,11	0.77784D-5 6,18	0.48878D-6 12,36	0.30810D-7 24,72

Positions are shown by space steps.

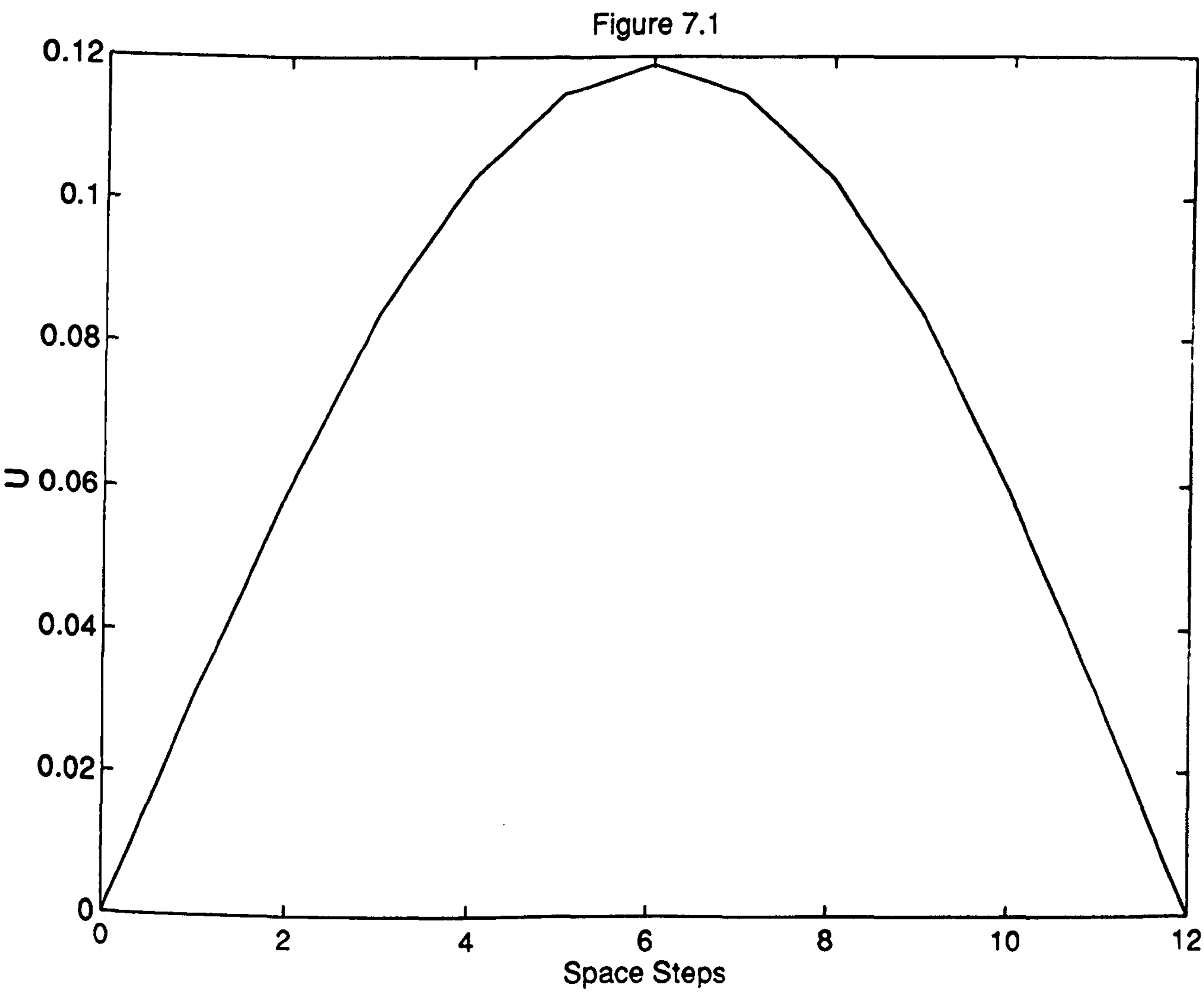

Figure 7.1: Numerical solution of example 1 for $h, l = \frac{1}{12}$ at time t=1.0

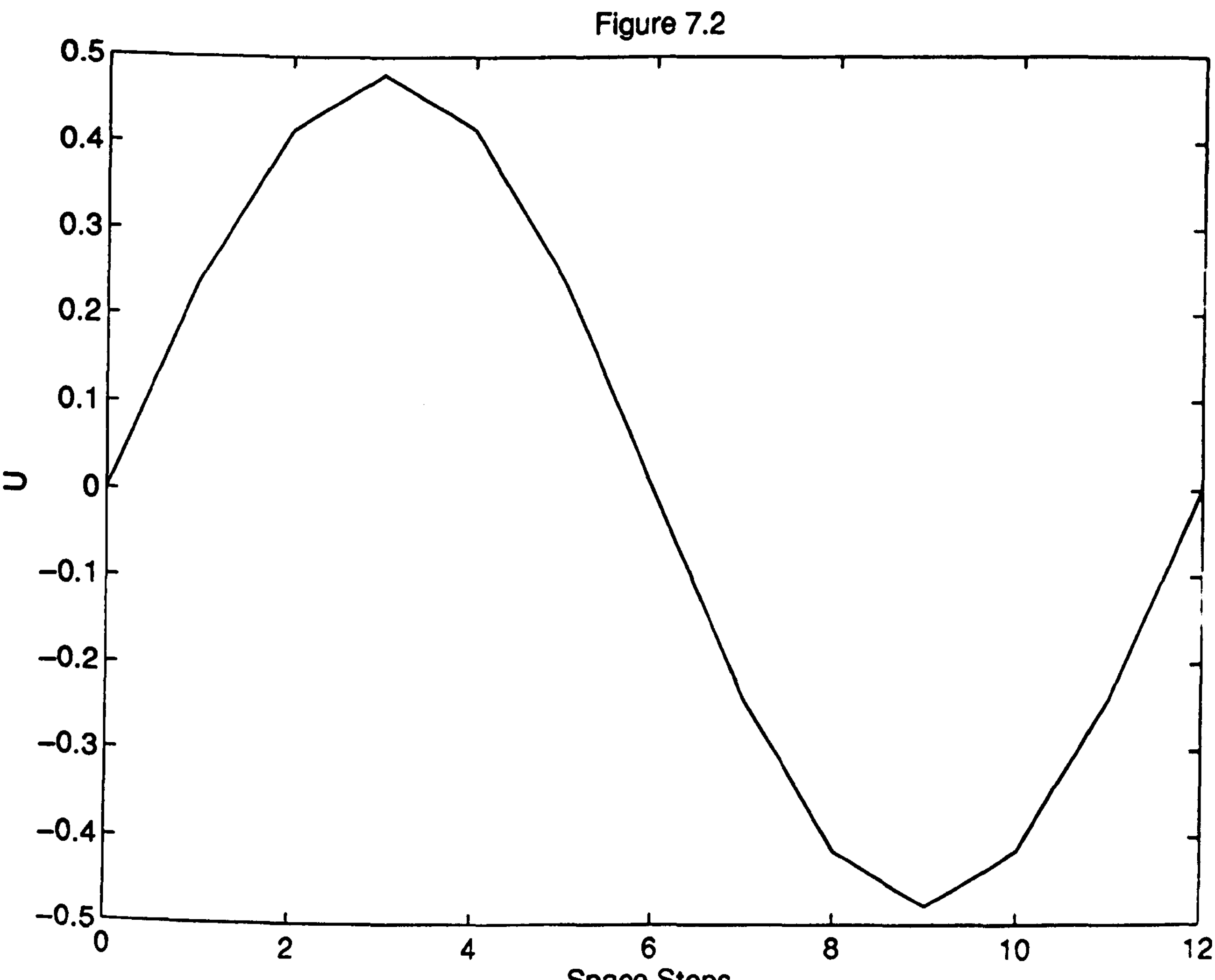

Figure 7.2: Numerical solution of example 1 for $h, l = \frac{1}{24}$ at time t=0.5

Chapter 8

Summary and Conclusions

8.1 Summary

The main theme of this thesis was to find some new numerical methods which are stable, require only real arithmetic and are third- or fourth-order accurate in space and time for parabolic/ hyperbolic partial differential equations and to develop parallel algorithms for their implementation.

Chapter 1 was written for introductory purposes and covers some general topics. For example, a basic introduction is given in Section 1.1, an introduction to the method of lines, very important in solving time-dependent partial differential equations, is given in Section 1.2, important notations are mentioned in Section 1.3, rational approximations to $exp(t)$ are mentioned in Section 1.4 and some mathematical properties of finite-difference methods, for example, error analysis, consistency, stability and convergence, are outlined in Section 1.5.

In Chapter 2 a family of third-order numerical methods for the advection equation with constant coefficients was developed. In Section 2.2, the model problem is outlined and third-order accuracy in the space component is achieved at all points of the space discretization in Section 2.3 and a new governing matrix was obtained. The third-order accuracy in the complementary component is also obtained using a rational approximation to the matrix exponential function, which can be resolved imto partial fractions, in Section 2.3. Since efficiency is also an important object of this thesis, a parallel algorithm which is implementable on an architecture consisting of three processors is developed in Section 2.4. This chapter is concluded by numerical examples which show that the methods are very effective. Pictorial evidence is also appended for support. This method is also modified for a non-linear problem in Section 2.6 and tested on a numerical example.

In Chapter 3 a family of fourth-order numerical methods for the advection equation, with constant coefficients, subject to some boundary conditions, is introduced. Fourth-order accuracy in the space component at all points of the space discretization is derived in Section 3.1 and a new matrix is obtained. A rational approximation, involving three parameters, is used to achieve fourth-order accuracy in the time variable. A parallel algorithm which is implementable on an architecture consisting of four processors is developed in Section 3.2. At the end of this chapter the same numerical examples, which are given in Chapter 2, are considered and it is found that numerical results are very accurate. Two numerical results are compared with latest research and depicted for pictorial evidence.

A family of third-order numerical methods is developed for the linear advection-diffusion equation in Chapter 4. Derivation of the methods is outlined in Section 4.2 in which the matrix exponential function is approximated by the rational approximation introduced in Section 1.3 of Chapter 1. Since most of the mathematics needed in this section is concerned in solving a system of linear equations so it was not presented in detail. In Section 4.3, a parallel algorithm was developed and presented in tabular form in Table 4.1. This algorithm is suitable for an architecture consisting of three processors. In Section 4.4 a representative of these methods is used to find numerical solution of a problem. The analytical and numerical solutions are depicted at the end of the chapter.

Considering again the model problem, discussed in Section 4.1, a family of fourth-order numerical methods is developed in Chapter 5. Derivation of the methods is outlined in Section 5.1 in which the matrix exponential function is approximated by the rational approximation introduced in Section 1.3. Once again only essential steps are presented in this section. In Section 5.2 a parallel algorithm was developed and presented in tabular form in Table 5.1. This algorithm is suitable for an architecture consisting of four processors. In Section 5.3 a representative of these methods is used to find numerical solutions of the problem given in Chapter 4. The numerical solution is graphed and appended at the end of this chapter.

A family of third-order numerical methods is developed for the linear, second-order wave equation in Chapter 6. The model problem is outlined in Section 6.1 and the method is derived in Section 6.3 in which the matrix exponential function is approximated again by the rational approximation introduced in Section 1.3 of Chapter 1. In Section 6.6, a parallel algorithm was developed and presented in tabular form in Table 6.1. This algorithm is suitable for an architecture consisting of at least three processors. In Section 6.7 a representative of these methods is used to find numerical solutions of two different problems. The analytical and some numerical solutions are depicted at the end of the chapter.

Considering again the model problem, discussed in Section 6.1, a family of fourth-order numerical methods is developed in Chapter 7. Derivation of the methods is outlined in Section 7.1 in which the matrix exponential function is approximated by the rational approximation introduced in Section 1.3. In Section 7.4 accuracy is shown to be fourth-order and in Section 7.5 a parallel algorithm is developed and presented in tabular form in Table 7.1. This algorithm suitable for an architecture consisting of at least four processors needs the solution at first time-step in different way which is outlined in Section 7.2. In Section 7.6 a representative of these methods is used to find numerical solutions of the problems given in Chapter 6. Two numerical solutions are graphed and appended at the end of the chapter.

It has been shown that all the numerical methods developed for all the problems discussed have a number of advantages over existing methods. The development of each method ensures that the high-order accuracy is maintained at mesh points adjacent to the boundaries of the region of integration. To overcome the resulting increase in bandwidth of the governing matrix, a pre-elimination routine can be used. The other main advantage of the methods is that they require the use of only real arithmetic, compared to the need of competing methods to use complex arithmetic in their implementation [4,5].

8.2 Conclusions

Up-to-now there has been no numerical method which achieves higher-order accuracy in time and the space variable. So the work considered in this thesis regarded as a first attempt in this direction. I believe that this work is a major contribution to the existing research.

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