Higher Order Parallel Splitting Methods for Parabolic Partial Differential Equations

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To

my wife Tasleem Akhter Cheema,

our sons, Shozab Ali and Tansheet Ali

and daughter Aisha Tasneem

who probably suffered more than I did.

Abstract

The thesis develops two families of numerical methods, based upon new rational approximations to the matrix exponential function, for solving second-order parabolic partial differential equations. These methods are L-stable, third- and fourth-order accurate in space and time, and do not require the use of complex arithmetic. In these methods second-order spatial derivatives are approximated by new difference approximations. Then parallel algorithms are developed and tested on one-, two- and three-dimensional heat equations, with constant coefficients, subject to homogeneous boundary conditions with discontinuities between initial and boundary conditions. The schemes are seen to have high accuracy.

A family of cubic polynomials, with a natural number dependent coefficients, is also introduced. Each member of this family has real zeros.

Third- and fourth-order methods are also developed for one-dimensional heat equation subject to time-dependent boundary conditions, approximating the integral term in a new way, and tested on a variety of problems from the literature.

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Chapter 1

Preliminaries

1.1 Introduction

Partial differential equations and systems of such equations appear in the description of physical processes. For example, in hydrodynamics, the theory of elasticity, the theory of electromagnetism, field of heat flow, diffusion of materials and quantum mechanics Gerald and Wheatley (1994). The solutions of the equations describe possible physical reactions that have to be fixed through boundary conditions, which may be of quite a different character. These equations involve two or more independent variables that determine the behaviour of the dependent variable as described by a differential equation, usually of second or higher order.

In the last two decades much attention has been given in the literature to the development of L_0-stable and accurate methods for the numerical solutions of second-order parabolic partial differential equations. For example, Lawson and Morris (1978) developed a second-order L_0-stable methodas an extrapolation of a first-order backward difference method in one- and two-space dimensions. This idea was developed further for one-space variable by Gourlay and Morris (1980) who achieved third- and fourth-order accuracy in time by a novel multistage process. The second-order method of Lawson and Morris (1978), was adapted and used in a practical problem involving a non-linear parabolic equation by Twizell and Smith (1982). Lawson and Swayne (1976) discussed a second-order accurate L_0-stable method for the heat conduction problem with time-dependent boundary conditions.

The general quasilinear partial differential equation of the second-order in two independent variables x and t has the form

$$a\frac{\partial^2 u}{\partial x^2} + b\frac{\partial^2 u}{\partial x \partial t} + c\frac{\partial^2 u}{\partial t^2} = e \qquad (1.1)$$

where $u = u(x,t)$ and a, b, c and e are functions of $x, t, u, \frac{\partial u}{\partial x}$ and $\frac{\partial u}{\partial t}$, but not of the second-order derivatives. This equation is said to be:

(i) *elliptic* when $b^2 - 4ac < 0$,

(ii) *parabolic* when $b^2 - 4ac = 0$, and

(iii) *hyperbolic* when $b^2 - 4ac > 0$.

This thesis is concerned only with second-order parabolic partial differential equations, in one-, two-, and three-space variables subject to homogeneous boundary conditions and in one-space variable subject to time-dependent boundary conditions.

1.2 Method of Lines

Covering the region, in which a numerical solution to be examined, by a rectangular grid with sides parallel to the axes and then replacing the spatial derivatives in the *PDE* by their finite-difference approximations is called a method of lines. Time dependent problems in Partial Differential Equations (PDEs) are often solved by the Method of Lines (MOL). By this method we can transform the initial/boundary-value problems into a system of ordinary differential equations which can be written in the matrix form as

$$\frac{d\mathbf{U}(t)}{dt} = A\mathbf{U}(t) + \mathbf{v}(t), \qquad (1.2)$$

where A is a square matrix, $\mathbf{v}(t)$ results from the non-homogeneous boundary-conditions and $\mathbf{U}$ is the solution vector at time t. It is easy to show that the solution $\mathbf{U}(t)$ of (1.2) satisfies the recurrence relation

$$\mathbf{U}(t+l) = exp(lA)\mathbf{U}(t) + \int_t^{t+l} exp((t+l-s)A)\mathbf{v}(s)ds; \quad t = 0, l, 2l, \ldots. \qquad (1.3)$$

Numerical methods are developed by approximating the exponential matrix function and integral term in this recurrence relation.

When boundary conditions are homogeneous $\mathbf{v}$ becomes zero and the recurrence relation (1.3) takes the form

$$\mathbf{U}(t+l) = exp(lA)\mathbf{U}(t); \quad t = 0, l, 2l, \ldots. \qquad (1.4)$$

Several exiting algorithms for the numerical solution are generated through an approximation to the matrix exponential function appearing in (1.4). The rational functions are frequently used for this purpose (see, for example, Fairweather (1978), Mitchell and Griffiths (1980), Reusch *et al.* (1988), Serbin (1985, 1992), Twizell *et al.* (1993) and Yevick *et al.* (1992)) Perhaps the most well known are the Padé approximations; for example, Reusch *et al.* (1988) have developed algorithms corresponding to high order factorized diagonal Padé approximations for parabolic PDE's which are no more complicated to implement than that corresponding to the Crank-Nicolson method (Voss and Khaliq, (1995)), Zakian (1971) used a partial fraction expansion to compute the matrix exponential function via Padé approximations which is particularly useful in parallel processing. But the methods corresponding to high order Padé approximations involve the square and higher powers of matrix A which incur high cost or use complex arithmetic which cause accumulated rounf off error. On the other hand Norsett and Wolfbrandt (1977) considered rational approximations to the exponential function with only real poles and showed that those with the smallest error constant occurred in the case of repeated poles. Lawson and Swayne (1976) developed a simple efficient algorithm for one dimensional parabolic PDE's using a second order rational approximation possessing one pole of multiplicity two , however,it lacks natural parallelism. Voss and Khaliq (1995) considered second order ratinal approximations which possess real and distinct poles and the resulting algorithms admitted parallelization through a real partial fraction expansion. At last but not least Twizell *et al.* (appearing in 1996) developed a family of second order methods which are L_0-stable and don't require complex arithmetic.

1.3 Motivation and Aims

The demands of both the scientific and the commercial communities for ever increasing computing power led to dramatic improvements in computer architecture. Initial efforts concentrated on achieving high performance on a single processor, but the more recent past has been witness to attempts to harness multiple processors. Multiprocessor systems consist of a number of interconnected processors each of which is capable of performing complex tasks independently of the others. In a sequential algorithm all processes are performed by a single processor turn by turn but in a parallel algorithm indepedent parts of the program are performed by different processors simultaneously which save a lot of time. So in this thesis parallel algorithms, which do not require complex arithmetic, will be developed and tested on heat equation with constant coefficients, subject to homogeneous boundary conditions and time-dependent boundary conditions, with discontinuities between initial and boundary conditions. Higher accuracy and L-stability are also important aims of this thesis.

1.4 Notations

Usually the theoretical solution of a parabolic 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 parabolic 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.

1.5 Analysis of Difference Schemes

1.5.1 Local Truncation Error

Suppose that a parabolic 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 the Taylor expansions about (mh, nl), the value of $l^{-1}F_{m,n}(u) - L(u_m^n)$ is the **local truncation error** at the mesh point (mh, nl) i.e; the local truncation error is the difference between the finite-difference scheme and the differential equation it is replacing.

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 parabolic equation is **consistent** if

$$local \quad truncation \quad error \longrightarrow 0$$

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 and computed solutions of the difference equation remains bounded as n increases, l remaining fixed for all m.

There are two methods which are commonly used for examining this notion of stability of a finite difference scheme.

(a) The von Neumann Method

Consider the local discretization error

$$\mathbf{Z}_m^n = \mathbf{U}_m^n - \tilde{\mathbf{U}}_m^n$$

and introduce the error function at a given time level t

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

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

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

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

$$e^{\alpha n l} e^{i\beta m h}.$$

The original error component $e^{i\beta m h}$ will not grow with time if

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

for all α. This is von Neumann's 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

$$A_n \mathbf{U}^{n+1} = B_n \mathbf{U}^n$$

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

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

and A_n, B_n are square matrices of order N. The above equation can be written in the form

$$\mathbf{U}^{n+1} = C_n \mathbf{U}^n$$

where $C_n = A_n^{-1} B_n$, provided $| A_n | \neq 0$. The error vector

$$\mathbf{Z}^n = \mathbf{U}^n - \tilde{\mathbf{U}}^n$$

satisfies

$$\mathbf{Z}^{n+1} = C_n \mathbf{Z}^n$$

from which it follows that

$$\| \mathbf{Z}^{n+1} \| \leq \| C_n \| \| \mathbf{Z}^n \|,$$

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

$$\| C_n \| \leq 1,$$

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

$$\| C_n \|_2 = \max_s | \lambda_s |$$

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

1.5.5 Alternative Definition of Stability

In general, numerical methods are of the form

$$\mathbf{U}^{n+1} = R(lA)\mathbf{U}^n, \quad n = 0, 1, 2, \ldots \tag{1. 5}$$

where $R(lA)$ is some approximation to $exp(lA)$ in (1.4). So the matrix method requires

$$\| R(lA) \|_s \leq 1.$$

This is equivalent to requiring

$$\mid R(l\lambda_s) \mid \leq 1$$

where λ_s is an eigenvalue of A. If the eigenvalues are negative and real then $l\lambda_s < 0$ and so $z = -l\lambda_s > 0$. Hence stability requires

$$\mid R(-z) \mid \leq 1.$$

Here the term $R(-z)$ is called the amplification symbol or symbol of the resulting numerical method.

Definition-1

If

$$\mathbf{U}^{n+1} = R(lA)\mathbf{U}^n, \quad n = 0, 1, 2, \ldots$$

where A is a matrix of order N with negative real eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_N$, the resulting finite-difference method is said to be A_0-**stable** if

$$\| R(lA) \|_s \leq 1$$

or

$$| R(-z) | \leq 1$$

where $z = -l\lambda_s$. A_0-stability corresponds to unconditional stability in the von Neumann sense.

Definition-2

An A_0-stable method for which, additionally,

$$\lim_{z \to \infty} R(-z) = 0$$

give rise to a finite-difference method which is L_0-**stable**.

Note:- If eigenvalues are complex with negative real parts then method is said to be L-acceptable.

1.5.6 Convergence

A finite-difference method for parabolic 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 $h, l \to 0$ simultaneously.

1.6 Solving a cubic equation

Consider the cubic equation

$$1 - ax + bx^2 - cx^3 = 0 \qquad (1.6)$$

which can be written as

$$x^3 - \frac{b}{c}x^2 + \frac{a}{c}x - \frac{1}{c} = 0. \qquad (1.7)$$

Repacing x by $y + \frac{b}{3c}$ in (1.7) gives

$$y^3 + \left(\frac{a}{c} - \frac{b^2}{3c^2}\right) y + \left(\frac{ab}{3c^2} - \frac{2b^3}{27c^3} - \frac{1}{c}\right) = 0. \tag{1. 8}$$

Now substituting $y = r\,cos(\theta)$ in (1.8) yields

$$r^3 cos^3(\theta) + \left(\frac{a}{c} - \frac{b^2}{3c^2}\right) r\,cos(\theta) = -\frac{ab}{3c^2} + \frac{2b^3}{27c^3} + \frac{1}{c}. \tag{1. 9}$$

Comparing (1.9) with

$$4cos^3(\theta) - 3cos(\theta) = cos(3\theta) \tag{1. 10}$$

gives

$$\frac{r^3}{4} = \frac{(3ac - b^2)r}{-9c^2} = \frac{2b^3 - 9abc + 27c^2}{27c^3 cos(3\theta)}. \tag{1. 11}$$

When $r \neq 0$ the left hand equality gives

$$r = \pm\frac{2}{3c}\sqrt{b^2 - 3ac}. \tag{1. 12}$$

So r has positive real values if

$$b^2 - 3ac > 0 \tag{1. 13}$$

Now from right hand equality

$$cos(3\theta) = \frac{2b^3 - 9abc + 27c^2}{3c(b^2 - 3ac)r}. \tag{1. 14}$$

Using (1.12) in (1.14) gives

$$cos(3\theta) = \frac{2b^3 - 9abc + 27c^2}{2c(b^2 - 3ac)^{\frac{3}{2}}}. \tag{1. 15}$$

So real values of θ are possible if

$$\left| \frac{2b^3 - 9abc + 27c^2}{2c(b^2 - 3ac)^{\frac{3}{2}}} \right| \leq 1. \tag{1. 16}$$

Then

$$\theta = \frac{2k\pi}{3} \pm \frac{1}{3} cos^{-1}\left(\frac{2b^3 - 9abc + 27c^2}{2c(b^2 - 3ac)^{\frac{3}{2}}}\right); \quad k = 0, 1, 2. \tag{1.17}$$

Consequently roots of (1.6) are given by

$$x = \frac{b}{3c} + r\,cos(\theta) \tag{1.18}$$

in which r and θ are defined by (1.12) and (1.17) respectively.

Chapter 2

Third-Order Numerical Methods

2.1 The Method

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

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

with the boundary conditions

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

and the initial condition

$$u(x,0) = g(x), \quad 0 \leq x \leq X \tag{2. 3}$$

where $g(x)$ is a given continuous function of x.

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

$$g(0) \neq 0 \quad or \quad g(X) \neq 0.$$

The solution of the problem $\{(2.1)\text{–}(2.3)\}$ gives the temperature u at a distance x units of length from one end of a thermally insulated thin bar after t units of time of heat conduction.

2.1.1 Discretization

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

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

($m = 0, 1, 2, \ldots, N, N+1$ 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 $t = 0$.

2.1.2 Transformation of {(2.1)-(2.3)} into a System of ODE's

To approximate the space derivative in (2.1) to third-order accuracy at some general point (x, t) of the mesh, assume that it may be replaced by the five-point formula

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

As this approximation is not symmetric, five points *are* needed.

Expanding the terms $u(x-h,t)$, $u(x+h,t)$, $u(x+2h,t)$ and $u(x+3h,t)$ about (x,t) in (2.4) gives

$$h^2\frac{\partial^2 u(x,t)}{\partial x^2} = (a+b+c+d+e)\,u(x,t)$$

$$
\begin{aligned}
&+ \quad (-a+c+2d+3e)\,h\frac{\partial u(x,t)}{\partial x} \\
&+ \quad \frac{1}{2!}(a+c+4d+9e)\,h^2\frac{\partial^2 u(x,t)}{\partial x^2} \\
&+ \quad \frac{1}{3!}(-a+c+8d+27e)\,h^3\frac{\partial^3 u(x,t)}{\partial x^3} \\
&+ \quad \frac{1}{4!}(a+c+16d+81e)\,h^4\frac{\partial^4 u(x,t)}{\partial x^4} \\
&+ \quad \frac{1}{5!}(-a+c+32d+243e)\,h^5\frac{\partial^5 u(x,t)}{\partial x^5} \\
&+ \quad \dots \qquad (2.5)
\end{aligned}
$$

Equating powers of $h^i (i = 0, 1, 2, 3, 4)$ in (2.5) gives

$$
\begin{aligned}
a+b+c+d+e &= 0, \\
-a+c+2d+3e &= 0, \\
a+c+4d+9e &= 2, \qquad (2.6) \\
-a+c+8d+27e &= 0, \\
a+c+16d+81e &= 0.
\end{aligned}
$$

The solution of the linear system (2.6) is

$$
a = \frac{11}{12}, \quad b = \frac{-5}{3}, \quad c = \frac{1}{2}, \quad d = \frac{1}{3}, \quad e = \frac{-1}{12} \qquad (2.7)
$$

so that

$$
\begin{aligned}
\frac{\partial^2 u(x,t)}{\partial x^2} &= \frac{1}{12h^2}\{11\,u(x-h,t) - 20\,u(x,t) + 6\,u(x+h,t) \\
&+ \quad 4\,u(x+2h,t) - u(x+3h,t)\} + \frac{h^3}{12}\frac{\partial^5 u(x,t)}{\partial x^5} \\
&+ \quad O(h^4)\, as \;\; h \to 0 \qquad (2.8)
\end{aligned}
$$

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

Equation (2.8) is valid only for $(x, t) = (x_m, t_n)$ with $m = 1, 2, \dots, N-2$. To attain the same accuracy at the end points (x_{N-1}, t_n) and (x_N, t_n), special formulae must be developed which approximate $\partial^2 u(x,t)/\partial x^2$ not only to third order but also with dominant error term $\frac{1}{12}h^3\partial^5 u(x,t)/\partial x^5$ for $x = x_{N-1}, x_N$ and $t = t_n$. To achieve both of these, six-point formulae will be needed in each case. It will also be useful (for example, for extrapolation) to retain the factor $(12h^2)^{-1}$ as in (2.8), as may be seen in (2.13) below.

Consider, then, the approximation to $\partial^2 u(x,t)/\partial x^2$ at the point $(x,t) = (x_{N-1}, t_n)$: let

$$\begin{aligned} 12\,h^2 \frac{\partial^2 u(x,t)}{\partial x^2} &= a\,u(x-3h,t) + b\,u(x-2h,t) + c\,u(x-h+h,t) \\ &+ d\,u(x,t) + e\,u(x+h,t) + f\,u(x+2h,t) \\ &+ h^5 \frac{\partial^5 u(x,t)}{\partial x^5}. \end{aligned} \tag{2.9}$$

Then

$$\begin{aligned} 12h^2 \frac{\partial^2 u(x,t)}{\partial x^2} &= (a+b+c+d+e+f)\,u(x,t) \\ &+ (-3a-2b-c+e+2f)\,h\frac{\partial u(x,t)}{\partial x} \\ &+ \frac{1}{2!}(9a+4b+c+e+4f)\,h^2\frac{\partial^2 u(x,t)}{\partial x^2} \\ &+ \frac{1}{3!}(-27a-8b-c+e+8f)\,h^3\frac{\partial^3 u(x,t)}{\partial x^3} \\ &+ \frac{1}{4!}(81a+16b+c+e+16f)\,h^4\frac{\partial^4 u(x,t)}{\partial x^4} \\ &+ \frac{1}{5!}(-243a-32b-c+e+32f)\,h^5\frac{\partial^5 u(x,t)}{\partial x^5} \\ &+ h^5\frac{\partial^5 u(x,t)}{\partial x^5} + \dots \end{aligned} \tag{2.10}$$

Equating powers of $h^i (i = 0,1,2,3,4,5)$ in (2.10) gives

$$\begin{aligned} a+b+c+d+e+f &= 0, \\ -3a-2b-c+e+2f &= 0, \\ 9a+4b+c+e+4f &= 24, \end{aligned}$$

$$\begin{aligned}
-27a - 8b - c + e + 8f &= 0, \qquad (2.11)\\
81a + 16b + c + e + 16f &= 0,\\
-243a - 32b - c + e + 32f &= -120.
\end{aligned}$$

The solution of the linear system (2.11) is

$$a = 1, \quad b = -6, \quad c = 26, \quad d = -40, \quad e = 21, \quad f = -2 \qquad (2.12)$$

so that, at the mesh point (x_{N-1}, t_n), the desired approximation to $\frac{\partial^2 u(x,t)}{\partial x^2}$ is

$$\begin{aligned}
\frac{\partial^2 u(x,t)}{\partial x^2} &= \frac{1}{12h^2}\{u(x-3h,t) - 6\,u(x-2h,t) + 26\,u(x-h,t) - 40\,u(x,t)\\
&+ 21\,u(x+h,t) - 2u(x+2h,t)\} + \frac{h^3}{12}\frac{\partial^5 u(x,t)}{\partial x^5}\\
&+ O(h^4)\, as \quad h \to 0 \qquad (2.13)
\end{aligned}$$

Suppose, now, that at the point $(x,t) = (x_N, t_n)$ the approximation to the second-order space derivative $\partial^2 u(x,t)/\partial x^2$ is given by

$$\begin{aligned}
12\,h^2\frac{\partial^2 u(x,t)}{\partial x^2} &= a\,u(x-4h,t) + b\,u(x-3h,t) + c\,u(x-2h,t)\\
&+ d\,u(x-h+h,t) + e\,u(x,t) + f\,u(x+h,t)\\
&+ h^5\frac{\partial^5 u(x,t)}{\partial x^5}. \qquad (2.14)
\end{aligned}$$

Then

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

$$
\begin{aligned}
&+ \quad \frac{1}{5!}(-1024a - 243b - 32c - d + f)\, h^5 \frac{\partial^5 u(x,t)}{\partial x^5} \\
&+ \quad h^5 \frac{\partial^5 u(x,t)}{\partial x^5} + \ldots
\end{aligned} \qquad (2.15)
$$

and equating powers of $h^i (i = 0, 1, 2, 3, 4, 5)$ in (2.15) gives

$$
\begin{aligned}
a + b + c + d + e + f &= 0, \\
-4a - 3b - 2c - d + f &= 0, \\
16a + 9b + 4c + d + f &= 24, \\
-64a - 27b - 8c - d + f &= 0, \\
256a + 81b + 16c + d + f &= 0, \\
-1024a - 243b - 32c - d + f &= -120.
\end{aligned} \qquad (2.16)
$$

The solution of the linear system (2.16) is

$$
a = 2, \quad b = -11, \quad c = 24, \quad d = -14, \quad e = -10, \quad f = -9. \qquad (2.17)
$$

Hence, at the mesh point (x_N, t_n), the approximation to $\partial^2 u(x,t)/\partial x^2$ is

$$
\begin{aligned}
\frac{\partial^2 u(x,t)}{\partial x^2} &= \frac{1}{12h^2}\{2\, u(x-4h,t) - 11\, u(x-3h,t) + 24\, u(x-2h,t) \\
&- \quad 14\, u(x-h,t) - 10\, u(x,t) - 9\, u(x+h,t)\} + \frac{h^3}{12}\frac{\partial^5 u(x,t)}{\partial x^5} \\
&+ \quad O(h^4)\, as \quad h \to 0
\end{aligned} \qquad (2.18)
$$

Applying (2.1) with (2.8), (2.13) and (2.18) to the mesh points of the grid at time level $t = t_n$ produces a system of ODE's of the form

$$
\frac{d\mathbf{U}(t)}{dt} = A\mathbf{U}(t), \quad t > 0 \qquad (2.19)
$$

with initial distribution

$$
\mathbf{U}(0) = \mathbf{g} \qquad (2.20)
$$

in which $\mathbf{U}(t) = [U_1(t), U_2(t), \ldots, U_N(t)]^T$, $\mathbf{g} = [g(x_1), g(x_2), \ldots, g(x_N)]^T$, T denoting transpose and

$$A = \frac{1}{12h^2}\begin{bmatrix} -20 & 6 & 4 & -1 & & & & \bigcirc \\ 11 & -20 & 6 & 4 & -1 & & & \\ & 11 & -20 & 6 & 4 & -1 & & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & & 11 & -20 & 6 & 4 & -1 \\ & & & & 11 & -20 & 6 & 4 \\ & & & 1 & -6 & 26 & -40 & 21 \\ \bigcirc & & & 2 & -11 & 24 & -14 & -10 \end{bmatrix}_{N\times N} \qquad (2.21)$$

It is observed that the matrix h^2A has distinct eigenvalues with negative real parts for N=7, 9, 19 and 39 given in Appendix A. Solving (2.19) subject to (2.20) gives the solution

$$\mathbf{U}(t) = exp(lA)\mathbf{U}(0) \qquad (2.22)$$

which satisfies the recurrence relation

$$\mathbf{U}(t+l) = exp(lA)\mathbf{U}(t), \quad t = 0, l, 2l, \ldots. \qquad (2.23)$$

2.2 A New Rational Approximant for $exp(lA)$

To approximate the matrix exponential function in (2.23), a new rational approximant, for a real scalar θ, given by

$$E_M(\theta) = \frac{\sum_{k=0}^{M-1} b_k\theta^k}{\sum_{k=0}^{M} a_k(-\theta)^k} \qquad (2.24)$$

is introduced, where M is a positive integer and $a_0 = 1$, $a_M, b_{M-1} \neq 0$ and $a_k \geq 0$ for all $k = 1, 2, 3, \ldots, M$. A particular case is $E_1(\theta)$ which is the (1,0) Padé approximant and $E_2(\theta)$ is discussed in Twizell *et al.* (1996). Matching $E_M(\theta)$ with the first $M+1$ terms of the Maclaurin expansion of $exp(\theta)$ leads to the following relations in the parameters

$$a_M = (-1)^{M-1} \sum_{k=0}^{M-1} (-1)^k \frac{a_k}{(M-k)!} \qquad (2.25)$$

and

$$b_k = \sum_{i=0}^{k} (-1)^i \frac{a_i}{(k-i)!}, \quad k = 0, 1, 2, \ldots, M-1. \qquad (2.26)$$

The magnitude of the coefficient of the error term is

$$\mu_M = \sum_{k=0}^{M-1} \frac{(M-k)(-1)^{k+1} a_k}{(M-k+1)!}. \qquad (2.27)$$

The present chapter is only concerned with $E_3(\theta)$. So for $M = 3$

$$E_3(\theta) = \frac{b_0 + b_1\theta + b_2\theta^2}{a_0 - a_1\theta + a_2\theta^2 - a_3\theta^3}. \qquad (2.28)$$

where $b_0 = 1, b_1 = 1 - a_1, b_2 = \frac{1}{2} - a_1 + a_2$, and $a_3 = \frac{1}{6} - \frac{a_1}{2} + a_2$. Let

$$b_0 + b_1\theta + b_2\theta^2 = p(\theta) \qquad (2.29)$$

and

$$a_0 - a_1\theta + a_2\theta^2 - a_3\theta^3 = q(\theta). \qquad (2.30)$$

In this case

$$\mu_3 = -\frac{1}{8} + \frac{a_1}{3} - \frac{a_2}{2}. \qquad (2.31)$$

2.3 L-Stability

Let λ be an eigenvalue of the matrix A given by (2.21). Then the amplification symbol of the numerical method arising from (2.24) is (Twizell, 1984)

$$R(-z) = \frac{\sum_{k=0}^{M-1} b_k(-z)^k}{\sum_{k=0}^{M} a_k(z)^k}.$$

It can be written as

$$R(-z) = \frac{\sum_{k=0}^{M-1} a_k z^k - \sum_{k=1}^{M-1} [a_k - (-1)^k b_k] z^k}{\sum_{k=0}^{M} a_k z^k}$$

or

$$R(-z) = \frac{\sum_{k=0}^{M-1} a_k z^k - \sum_{k=1}^{M-1}[a_k - (-1)^k b_k] z^k}{\sum_{k=0}^{M-1} a_k z^k + a_M z^M} \qquad (2.\ 32)$$

where $z = -lRe(\lambda) > 0$. Thus L-stability is guaranteed (Twizell, 1984) provided

$$a_M > 0 \qquad (2.\ 33)$$

and

$$a_k - (-1)^k b_k \geq 0, \quad for\ all\ \ k = 1, 2, \ldots, M-1. \qquad (2.\ 34)$$

Using (2.26) in (2.34) gives

$$a_k - (-1)^k \sum_{i=0}^{k} (-1)^i \frac{a_i}{(k-i)!} \geq 0, \quad k = 1, 2, \ldots, M-1.$$

or

$$(-1)^{k-1} \sum_{i=0}^{k-1} (-1)^i \frac{a_i}{(k-i)!} \geq 0, \quad for\ all\ k = 1, 2, \ldots, M. \qquad (2.\ 35)$$

Particularly for $M = 3$, L-stability follows if

$$a_1 > \frac{1}{2} \qquad (2.\ 36)$$

and

$$a_2 > \frac{a_1}{2} - \frac{1}{6}. \qquad (2.\ 37)$$

2.4 Avoiding Complex Arithmetic

Complex arithmetic can be avoided in a numerical method if the denominator of the rational approximation has only real zeros. Unfortunately there is no formula to find the zeros of a polynomial of degree greater than 4 in closed form. So numerical methods must be used to find the zeros of higher-degree polynomials. This chapter is concerned only with the polynomials defined by (2.29) and (2.30). The denominator of $E_3(\theta)$, $q(\theta)$, has distinct real zeros (MacDuffee,(1954)) provided

$$a_2^2 - 3a_1a_3 > 0 \quad (2.38)$$

and

$$\left| \frac{2a_2^3 - 9a_1a_2a_3 + 27a_3^2}{2(a_2^2 - 3a_1a_3)^{\frac{3}{2}}} \right| \leq 1 \quad (2.39)$$

2.4.1 Availability of Real Zeros for $q(\theta)$

Taking

$$a_1 = \frac{n+15}{10}, \quad a_2 = \frac{3n+41}{60}$$

, where n is a natural number, gives

$$a_3 = \frac{1}{10}, \quad \mu_3 = \frac{n+4}{120}$$

and {(2.36)-(2.39)} hold for all n. Unfortunately $\mu_3 \to \infty$ as $n \to \infty$, so only small values of n are useful. Since the discriminant of $p(\theta)$, defined by (2.29), is also positive for all n so it can be factorized and a sequential algorithm involving no square or higher powers of A can be constructed. In addition to this combination a long list of values of a_1, a_2 and a_3 which satisfy the conditions {(2.36)-(2.39)} and produce real zeros for $q(\theta)$, defined by (2.30), is obtained. A few of these are given in Appendix B.

2.5 Algorithm 1

Suppose that a_1, a_2 and a_3 satisfy the conditions {(2.36)-(2.39)} and $r_i(i = 1, 2, 3)$ are distinct real zeros of $q(\theta)$ defined by (2.30) then

$$exp(lA) = \sum_{i=1}^{3} c_i \left(I - \frac{l}{r_i} A \right)^{-1} \quad (2.40)$$

where c_i $(i = 1, 2, 3)$, the partial-fraction coefficients of $E_3(\theta)$, are defined by

$$c_i = \frac{p(r_i)}{\prod^3_{\substack{j=1 \\ j \neq i}} \left(1 - \frac{r_i}{r_j}\right)}, \quad i = 1, 2, 3 \qquad (2.41)$$

So, using (2.40) in (2.23) gives

$$\mathbf{U}(t + l) = \left(\sum_{i=1}^{3} c_i \left(I - \frac{l}{r_i} A \right)^{-1} \right) \mathbf{U}(t). \qquad (2.42)$$

Let

$$c_i \left(I - \frac{l}{r_i} A \right)^{-1} \mathbf{U}(t) = \mathbf{w}_i(t), \quad i = 1, 2, 3, \qquad (2.43)$$

Then the systems of linear equations

$$\left(I - \frac{l}{r_i} A \right) \mathbf{w}_i(t) = c_i \mathbf{U}(t), \quad i = 1, 2, 3 \qquad (2.44)$$

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

$$\mathbf{U}(t + l) = \sum_{i=1}^{3} \mathbf{w}_i(t). \qquad (2.45)$$

This algorithm is given in tabular form in Table 2.2.

2.6 Extension to two-space dimensions

Consider the two-dimensional heat equation with constant coefficients

$$\frac{\partial u(x,y,t)}{\partial t} = \frac{\partial^2 u(x,y,t)}{\partial x^2} + \frac{\partial^2 u(x,y,t)}{\partial y^2}, \quad 0 < x, y < X, \ t > 0 \qquad (2.46)$$

subject to the initial conditions

$$u(x, y, 0) = g(x, y), \quad 0 \leq x, y \leq X \qquad (2.47)$$

where $g(x, y)$ is a continuous function of x and y and the boundary conditions

$$u(0, y, t) = u(X, y, t) = 0, \quad t > 0 \qquad (2.48)$$

$$u(x,0,t) = u(x,X,t) = 0, \quad t > 0. \tag{2.49}$$

Discretizing $0 \leq x, y \leq X$ as in the one-dimensional case using equal space steps and replacing the space derivatives in the PDE (2.46) by the appropriate third-order difference approximations{(2.8),(2.13),(2.18)} and applying to the all N^2-interior mesh points at time level $t = nl$ $(n = 1, 2, 3, \ldots)$ gives a system of N^2 first-order ordinary differential equations which may be written in matrix form as

$$\frac{d\mathbf{U}(t)}{dt} = A\mathbf{U}(t), \quad t > 0 \tag{2.50}$$

with

$$\mathbf{U}(0) = \mathbf{g}, \tag{2.51}$$

where $\mathbf{U}(t) = [U_{1,1}(t), U_{2,1}(t), \ldots, U_{N,1}(t), \ldots, U_{1,N}(t), U_{2,N}(t), \ldots, U_{N,N}(t)]^T$ and $\mathbf{g} = [g_{1,1}, g_{2,1}, \ldots, g_{N,1}, \ldots, g_{1,N}, g_{2,N}, \ldots, g_{N,N}]^T$, T denoting transpose. The matrix A is the sum of two square matrices B and C of order N^2, given by

$$B = \frac{1}{12h^2}\begin{bmatrix} B_1 & & & \\ & B_1 & & \\ & & \ddots & \\ & & & B_1 \end{bmatrix} \tag{2.52}$$

where

$$B_1 = \begin{bmatrix} -20 & 6 & 4 & -1 & & & & \bigcirc \\ 11 & -20 & 6 & 4 & -1 & & & \\ & 11 & -20 & 6 & 4 & -1 & & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & & 11 & -20 & 6 & 4 & -1 \\ & & & & 11 & -20 & 6 & 4 \\ & & & 1 & -6 & 26 & -40 & 21 \\ \bigcirc & & & 2 & -11 & 24 & -14 & -10 \end{bmatrix} \tag{2.53}$$

and

$$C = \frac{1}{12h^2}\begin{bmatrix} -20I & 6I & 4I & -I & & & & & \bigcirc \\ 11I & -20I & 6I & 4I & -I & & & & \\ & 11I & -20I & 6I & 4I & -I & & & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & & \\ & & & 11I & -20I & 6I & 4I & -I \\ & & & & 11I & -20I & 6I & 4I \\ & & & I & -6I & 26I & -40I & 21I \\ \bigcirc & & & 2I & -11I & 24I & -14I & -10I \end{bmatrix} \qquad (2.54)$$

where I is the identity matrix of order N. Clearly B and C commute. Solving (2.50) subject to the initial condition (2.51) gives (2.23).

2.6.1 Algorithm 2

Since $A = B + C$ and A and B commute, (2.23) becomes

$$\mathbf{U}(t+l) = exp(lB)exp(lC)\mathbf{U}(t), \quad t = 0, l, 2l, \ldots, \qquad (2.55)$$

to third order. Using (2.40) gives

$$exp(lB) = \sum_{i=1}^{3} c_i \left(I - \frac{l}{r_i}B\right)^{-1} \qquad (2.56)$$

and

$$exp(lC) = \sum_{i=1}^{3} c_i \left(I - \frac{l}{r_i}C\right)^{-1}. \qquad (2.57)$$

So (2.55) becomes

$$\mathbf{U}(t+l) = \left(\sum_{i=1}^{3} c_i \left(I - \frac{l}{r_i}B\right)^{-1}\right) \left(\sum_{i=1}^{3} c_i \left(I - \frac{l}{r_i}C\right)^{-1}\right) \mathbf{U}(t). \qquad (2.58)$$

Let

$$\mathbf{z}_i(t) = c_i \left(I - \frac{l}{r_i}C\right)^{-1} \mathbf{U}(t), \quad i = 1, 2, 3, \qquad (2.59)$$

then the systems

$$\left(I - \frac{l}{r_i}C\right) \mathbf{z}_i(t) = c_i\mathbf{U}(t), \quad i = 1, 2, 3, \tag{2. 60}$$

can be solved on three different processors simultaneously. Let

$$\mathbf{Z}(t) = \sum_{i=1}^{3} \mathbf{z}_i(t), \tag{2. 61}$$

then (2.58) has the form

$$\mathbf{U}(t+l) = \left(\sum_{i=1}^{3} c_i \left(I - \frac{l}{r_i}B\right)^{-1}\right) \mathbf{Z}(t) \tag{2. 62}$$

or

$$\mathbf{U}(t+l) = \sum_{i=1}^{3} \mathbf{w}_i(t) \tag{2. 63}$$

where $\mathbf{w}_i (i = 1, 2, 3)$, the solutions of the linear systems

$$\left(I - \frac{l}{r_i}B\right) \mathbf{w}_i(t) = c_i\mathbf{Z}(t), \quad i = 1, 2, 3, \tag{2. 64}$$

can be computed on three differet processors simultaneously. Here $\mathbf{z}_i$ and $\mathbf{w}_i (i = 1, 2, 3)$ are intermediate vectors of order N^2. This algorithm is given in tabular form in Table 2.3.

2.7 Extension to three-space dimensions

Consider the partial differential equation

$$\frac{\partial u(x,y,z,t)}{\partial t} = \frac{\partial^2 u(x,y,z,t)}{\partial x^2} + \frac{\partial^2 u(x,y,z,t)}{\partial y^2} + \frac{\partial^2 u(x,y,z,t)}{\partial z^2}, \tag{2. 65}$$

in the region $0 < x, y, z < X,\ t > 0$, subject to the initial condition

$$u(x,y,z,0) = g(x,y,z), \quad 0 \leq x, y, z \leq X \tag{2. 66}$$

where $g(x,y,z)$ is a continuous function of the space variables and the boundary conditions

$$u(0,y,z,t) = u(X,y,z,t) = 0, \quad 0 \le y,z \le X \quad t > 0 \qquad (2.67)$$

$$u(x,0,z,t) = u(x,X,z,t) = 0, \quad 0 \le x,z \le X \quad t > 0 \qquad (2.68)$$

$$u(x,y,0,t) = u(x,y,X,t) = 0, \quad 0 \le x,y \le X \quad t > 0. \qquad (2.69)$$

Discretizing $0 \le x,y,z \le X$ as in the one-dimensional case, using equal space steps in all directions, and replacing the space derivatives in the PDE (2.65) by the appropriate third-order difference approximations {(2.8), (2.13), (2.18)} and applying to all the N^3 interior mesh points at the time levels $t_n = nl$ $(n = 1,2,3,\ldots)$, leads to a system of N^3 first-order ordinary differential equations written in matrix form as

$$\frac{d\mathbf{U}(t)}{dt} = A\mathbf{U}(t), \quad t > 0 \qquad (2.70)$$

with

$$\mathbf{U}(0) = \mathbf{g}, \qquad (2.71)$$

where

$$\mathbf{U}(t) = [U_{1,1,1}(t), U_{2,1,1}(t), \ldots, U_{N,1,1}(t), U_{1,2,1}(t), U_{2,2,1}(t), \ldots, U_{N,N,N}(t)]^T$$

and $\mathbf{g} = [g_{1,1,1}, g_{2,1,1}, \ldots, g_{N,1,1}, g_{1,2,1}, g_{2,2,1}, \ldots, g_{N,N,N}]^T$, T denoting transpose. The square matrix A of order N^3 may be written as

$$A = A_1 + A_2 + A_3 \qquad (2.72)$$

where A_1, A_2 and A_3 result from the replacements of the space derivatives in (2.65) by the third-order difference approximations {(2.8), (2.13), (2.18)}. They are commutable and are given by

$$A_1 = \frac{1}{12h^2}\begin{bmatrix} B_1 & & & \\ & B_1 & & \\ & & \ddots & \\ & & & B_1 \end{bmatrix}, \qquad (2.73)$$

a block-diagonal matrix with N^2 diagonal blocks given by

$$B_1 = \begin{bmatrix} -20 & 6 & 4 & -1 & & & & & \bigcirc \\ 11 & -20 & 6 & 4 & -1 & & & & \\ & 11 & -20 & 6 & 4 & -1 & & & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & & \\ & & & 11 & -20 & 6 & 4 & -1 \\ & & & & 11 & -20 & 6 & 4 \\ & & & 1 & -6 & 26 & -40 & 21 \\ \bigcirc & & & 2 & -11 & 24 & -14 & -10 \end{bmatrix}_{N\times N}, \qquad (2.74)$$

$$A_2 = \frac{1}{12h^2}\begin{bmatrix} B_2 & & & \\ & B_2 & & \\ & & \ddots & \\ & & & B_2 \end{bmatrix} \qquad (2.75)$$

is a block-diagonal matrix with N diagonal blocks given by

$$B_2 = \begin{bmatrix} -20I & 6I & 4I & -I & & & & & \bigcirc \\ 11I & -20I & 6I & 4I & -I & & & & \\ & 11I & -20I & 6I & 4I & -I & & & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & & \\ & & & 11I & -20I & 6I & 4I & -I \\ & & & & 11I & -20I & 6I & 4I \\ & & & I & -6I & 26I & -40I & 21I \\ \bigcirc & & & 2I & -11I & 24I & -14I & -10I \end{bmatrix}_{N^2\times N^2} \qquad (2.76)$$

in which I is the identity matrix of order N, and

$$A_3 = \frac{1}{12h^2}\begin{bmatrix} -20I^* & 6I^* & 4I^* & -I^* & & & & & \bigcirc \\ 11I^* & -20I^* & 6I^* & 4I^* & -I^* & & & & \\ & 11I^* & -20I^* & 6I^* & 4I^* & -I^* & & & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & & \\ & & & 11I^* & -20I^* & 6I^* & 4I^* & -I^* \\ & & & & 11I^* & -20I^* & 6I^* & 4I^* \\ & & & I^* & -6I^* & 26I^* & -40I^* & 21I^* \\ \bigcirc & & & 2I^* & -11I^* & 24I^* & -14I^* & -10I^* \end{bmatrix}_{N^3\times N^3} \qquad (2.77)$$

where I^* is the identity matrix of order N^2. Solving (2.70) subject to the initial condition (2.71) gives (2.23).

2.7.1 Algorithm 3

Replacing A by $A_1 + A_2 + A_3$ in (2.23) gives, since A_1, A_2 and A_3 commute,

$$\mathbf{U}(t+l) = exp(lA_1)exp(lA_2)exp(lA_3)\mathbf{U}(t), \quad t = 0, l, 2l, \ldots. \tag{2. 78}$$

Using (2.40) gives

$$exp(lA_1) = \sum_{i=1}^{3} c_i \left(I - \frac{l}{r_i}A_1\right)^{-1}, \tag{2. 79}$$

$$exp(lA_2) = \sum_{i=1}^{3} c_i \left(I - \frac{l}{r_i}A_2\right)^{-1}, \tag{2. 80}$$

and

$$exp(lA_3) = \sum_{i=1}^{3} c_i \left(I - \frac{l}{r_i}A_3\right)^{-1}. \tag{2. 81}$$

So (2.78) becomes

$$\mathbf{U}(t+l) = \sum_{i=1}^{3} c_i \left(I - \frac{l}{r_i}A_1\right)^{-1} \sum_{i=1}^{3} c_i \left(I - \frac{l}{r_i}A_2\right)^{-1} \sum_{i=1}^{3} c_i \left(I - \frac{l}{r_i}A_3\right)^{-1} \mathbf{U}(t). \tag{2. 82}$$

Let

$$\mathbf{z}_i(t) = c_i \left(I - \frac{l}{r_i}A_3\right)^{-1} \mathbf{U}(t), \quad i = 1, 2, 3, \tag{2. 83}$$

then

$$\left(I - \frac{l}{r_i}A_3\right) \mathbf{z}_i(t) = c_i\mathbf{U}(t), \quad i = 1, 2, 3. \tag{2. 84}$$

Taking

$$\mathbf{Z}(t) = \sum_{i=1}^{3} \mathbf{z}_i(t), \tag{2. 85}$$

leads to

$$\mathbf{U}(t+l) = \sum_{i=1}^{3} c_i \left(I - \frac{l}{r_i}A_1\right)^{-1} \sum_{i=1}^{3} c_i \left(I - \frac{l}{r_i}A_2\right)^{-1} \mathbf{Z}(t). \tag{2. 86}$$

Let

$$\mathbf{y}_i(t) = c_i \left(I - \frac{l}{r_i}A_2\right)^{-1} \mathbf{Z}(t), \quad i = 1, 2, 3, \tag{2. 87}$$

then

$$\left(I - \frac{l}{r_i}A_2\right)\mathbf{y}_i(t) = c_i\mathbf{Z}(t), \quad i = 1, 2, 3. \tag{2.88}$$

Let

$$\mathbf{Y}(t) = \sum_{i=1}^{3}\mathbf{y}_i(t), \tag{2.89}$$

then (2.86) becomes

$$\mathbf{U}(t+l) = \sum_{i=1}^{3}\mathbf{w}_i(t), \tag{2.90}$$

where $\mathbf{w}_i (i = 1, 2, 3)$ are the solutions of the linear systems

$$\left(I - \frac{l}{r_i}A_1\right)\mathbf{w}_i(t) = c_i\mathbf{Y}(t), \quad i = 1, 2, 3. \tag{2.91}$$

Here {(2.84),(2.85),(2.88)–(2.91)} constitute the algorithm. Using this algorithm three different processors can be used simultaneously thrice. This algorithm is given in tabular form in Table 2.4.

2.8 Numerical Examples

In this section a representative of many other methods based on (2.28) will only be used. So taking

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

and

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

gives

$$a_3 = \frac{4143}{50000}, \quad b_1 = -\frac{15431}{50000}, \quad b_2 = -\frac{14287}{60000}$$

and then it is found that

$$r_1 = 2.1883713223893, \quad r_2 = 2.3398749224808, \quad r_3 = 2.3569013937170$$

are the real zeros of (2.30). Using these values in (2.41) gives

$$c_1 = -176.18490160503, \quad c_2 = 2051.1048759736, \quad c_3 = -1873.9199743685$$

According to these values of parameters the amplification symbol of the method is depicted in Fig. 2.1.

2.8.1 One-dimensional Problem

Example 1

Considering the one space dimensional heat equation with constant coefficients (2.1) and taking $X = 2$ and $g(x) = 1$ in $\{(2.1)\text{-}(2.3)\}$ the model problem becomes

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad 0 < x < 2, \quad t > 0 \qquad (2.92)$$

subject to the initial condition

$$u(x,0) = 1, \quad 0 \le x \le 2 \qquad (2.93)$$

and the boundary conditions

$$u(0,t) = u(2,t) = 0, \quad t > 0. \qquad (2.94)$$

This problem, which has theoretical solution

$$u(x,t) = \sum_{k=1}^{\infty} [1 - (-1)^k] \frac{2}{k\pi} sin(\frac{k\pi x}{2}) exp(-\frac{k^2\pi^2 t}{4}), \qquad (2.95)$$

(Lawson and Morris, 1978) has discontinuities between the initial conditions and the boundary conditrions at $x = 0$ and $x = 2$. The theoretical solution at time $t = 1.0$ is depicted in Figure 2.2.

Using Algorithm 1 the model problem $\{(2.92)\text{-}(2.94)\}$ is solved for l=0.125, 0.1, 0.05, 0.025, 0.0125, 0.01, 0.005 and 0.001, and h=0.25, 0.2, 0.1, 0.05, 0.025, 0.02, 0.01 and 0.001. and compared with the $O(h^2 + l^2)$ method of Twizell *et al.* (1996) taking $l = 0.1$ and h=0.1, 0.05, 0.025, 0.01, 0.001 as shown in Table 2.1. For these values of h, it may be verified using the NAG subroutine F02AJF that the matrix A, given by (2.21), has distinct eigenvalues with negative real parts so that the numerical method is L-acceptable. In these experiments the method behaves smoothly over the whole interval $0 \leq x \leq 2$. The numerical solution for $h = 0.1$ and $l = 0.1$ is depicted in Figure 2.3. All other numerical solutions produce similar graphs. Maximum errors with positions at the time $t = 1.0$ are given in Table 2.5.

Table 2.1: Comparison

Methods	h=0.1	h=0.05	h=0.025	h=0.01	h=0.001
$O(h^2 + l^2)$	0.6823D-3	0.9286D-3	0.9902D-3	0.1008D-2	0.1011D-2
$O(h^3 + l^3)$	0.9116D-4	0.9088D-4	0.9097D-4	0.9098D-4	0.9100D-4

2.8.2 Two-dimensional Problem

Example 2

Considering the two space dimensional heat equation with constant coefficients {(2.46)-(2.49)} with $X = 2$ and $g(x, y) = sin(\frac{\pi}{2}y)$ the model problem becomes

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial t^2} + \frac{\partial^2 u}{\partial t^2}, \quad 0 < x, y < 2, \quad t > 0 \qquad (2.96)$$

subject to the initial condition

$$u(x, y, 0) = sin(\frac{\pi y}{2}), \quad 0 \leq x, y \leq 2 \qquad (2.97)$$

and the boundary conditions

$$u(x, y, t) = 0, \quad t > 0 \qquad (2.98)$$

on the lines $x = 0$, $y = 0$, $x = 2$ and $y = 2$.

The initial distribution is shown in Figure 2.4 and the theoretical solution of the above problem

$$u(x,y,t) = sin(\frac{\pi}{2}y)\sum_{k=1}^{\infty}[1-(-1)^k]\frac{2}{k\pi}sin(\frac{k\pi x}{2})exp(-\frac{(k^2+1)\pi^2 t}{4}) \quad (2.\ 99)$$

given by Lawson and Morris (1978) is depicted at time $t = 1.0$ in Figure 2.5. The maximum value of u at time $t = 1.0$ occurs for $(x, y) = (1, 1)$ and is approximately 0.00915699.

Since the initial function does not necessarily have the value zero on the square, for example, $u(0, 1, 0) = 1$ discontinuities between initial condition and boundary conditions do exist.

Using Algorithm 2 the model problem {(2.96)–(2.98)} is solved for l=0.125, 0.1, 0.05, 0.025, 0.2, 0.0125, 0.01, 0.005, 0.001 and h=0.25, 0.2, 0.1, 0.05, 0.04, 0.025, 0.02, 0.01. The numerical solution for $h = 0.1$ and $l = 0.1$ is depicted in Figure 2.6. All other choices give similar graphs. In these experiments the method behaves smoothly over the whole interval $0 \leq x \leq 2$. Maximum errors, with positions, at the time $t = 1.0$ are given in Table 2.7.

2.8.3 Three-dimensional Problem

Example 3

Considering the three space dimensional heat equation with constant coefficients {(2.65)-(2.69)} with $X = 2$ and $g(x,y,z) = sin(\frac{\pi}{2}x)sin(\frac{\pi}{2}y)sin(\frac{\pi}{2}z)$ the model problem becomes

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial t^2} + \frac{\partial^2 u}{\partial t^2} + \frac{\partial^2 u}{\partial t^2}, \quad 0 < x, y, z < 2, \quad t > 0 \qquad (2.\ 100)$$

subject to the initial condition

$$u(x,y,z,0) = sin(\frac{1}{2}\pi x)sin(\frac{1}{2}\pi y)sin(\frac{1}{2}\pi z), \quad 0 \leq x,y,z \leq 2 \qquad (2.\ 101)$$

and the boundary conditions

$$u(x,y,z,t) = 0, \quad t > 0 \qquad (2.\ 102)$$

on the planes $x = 0$, $y = 0$, $z = 0$, $x = 2$, $y = 2$ and $z = 2$.

The theoretical solution of the above problem is

$$u(x,y,z,t) = sin(\frac{\pi}{2}x)sin(\frac{\pi}{2}y)sin(\frac{\pi}{2}z)exp(-\frac{3}{4}\pi^2 t). \qquad (2.\ 103)$$

The maximum value of u at time $t = 0.1$ occurs for $(x,y,z) = (1,1,1)$ and is approximately 0.37616 .

Using Algorithm 3 the model problem {(2.100)–(2.102)} is solved for $l = 0.0125, 0.01, 0.005, 0.0025, 0.001$ and h=0.25, 0.2, 0.1, 0.05. In these experiments the method behaves smoothly over the whole interval $0 \leq x,y,z \leq 2$. Maximum errors with positions at the time $t = 0.1$ are given in Table 2.9.

Table 2.2: 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 Solve	$L_1U_1\mathbf{w}_1(t)$ $= c_1\mathbf{U}(t)$	$L_2U_2\mathbf{w}_2(t)$ $= c_2\mathbf{U}(t)$	$L_3U_3\mathbf{w}_3(t)$ $= c_3\mathbf{U}(t)$
5	$\mathbf{U}(t+l) = \mathbf{w}_1(t) + \mathbf{w}_2(t) + \mathbf{w}_3(t)$		
6	GO TO Step 4 for next time step		

Table 2.3: Algorithm 2

Steps	Processor 1	Processor 2	Processor 3
1 Input	l, r_1, c_1 $\mathbf{U}_0, B, C$	l, r_2, c_2 $\mathbf{U}_0, B, C$	l, r_3, c_3 $\mathbf{U}_0, B, C$
2 Compute	$I - \frac{l}{r_1}B$ $I - \frac{l}{r_1}C$	$I - \frac{l}{r_2}B$ $I - \frac{l}{r_2}C$	$I - \frac{l}{r_3}B$ $I - \frac{l}{r_3}C$
3 Decompose	$I - \frac{l}{r_1}B$ $= L_1U_1$ $I - \frac{l}{r_1}C$ $= P_1Q_1$	$I - \frac{l}{r_2}B$ $= L_2U_2$ $I - \frac{l}{r_2}C$ $= P_2Q_2$	$I - \frac{l}{r_3}B$ $= L_3U_3$ $I - \frac{l}{r_3}C$ $= P_3Q_3$
4 Solve	$P_1Q_1\mathbf{z}_1(t)$ $= c_1\mathbf{U}(t)$	$P_2Q_2\mathbf{z}_2(t)$ $= c_2\mathbf{U}(t)$	$P_3Q_3\mathbf{z}_3(t)$ $= c_3\mathbf{U}(t)$
5	$\mathbf{Z}(t) = \mathbf{z}_1(t) + \mathbf{z}_2(t) + \mathbf{z}_3(t)$		
6 Solve	$L_1U_1\mathbf{w}_1(t)$ $= c_1\mathbf{Z}(t)$	$L_2U_2\mathbf{w}_2(t)$ $= c_2\mathbf{Z}(t)$	$L_3U_3\mathbf{w}_3(t)$ $= c_3\mathbf{Z}(t)$
7	$\mathbf{U}(t+l) = \mathbf{w}_1(t) + \mathbf{w}_2(t) + \mathbf{w}_3(t)$		
8	GO TO Step 4 for next time step		

Table 2.4: Algorithm 3

Steps	Processor 1	Processor 2	Processor 3
1 Input	$l, r_1, c_1, \mathbf{U}_0,$ A_1, A_2, A_3	$l, r_2, c_2, \mathbf{U}_0,$ A_1, A_2, A_3	$l, r_3, c_3, \mathbf{U}_0,$ A_1, A_2, A_3
2 Compute	$I - \frac{l}{r_1} A_1$ $I - \frac{l}{r_1} A_2$ $I - \frac{l}{r_1} A_3$	$I - \frac{l}{r_2} A_1$ $I - \frac{l}{r_2} A_2$ $I - \frac{l}{r_2} A_3$	$I - \frac{l}{r_3} A_1$ $I - \frac{l}{r_3} A_2$ $I - \frac{l}{r_3} A_3$
3 Decompose	$I - \frac{l}{r_1} A_3$ $= P_1 Q_1$ $I - \frac{l}{r_1} A_2$ $= F_1 G_1$ $I - \frac{l}{r_1} A_1$ $= L_1 U_1$	$I - \frac{l}{r_2} A_3$ $= P_2 Q_2$ $I - \frac{l}{r_2} A_2$ $= F_2 G_2$ $I - \frac{l}{r_2} A_1$ $= L_2 U_2$	$I - \frac{l}{r_3} A_3$ $= P_3 Q_3$ $I - \frac{l}{r_2} A_3$ $= F_3 G_3$ $I - \frac{l}{r_3} A_1$ $= L_3 U_3$
4 Solve	$P_1 Q_1 \mathbf{z}_1(t)$ $= c_1 \mathbf{U}(t)$	$P_2 Q_2 \mathbf{z}_2(t)$ $= c_2 \mathbf{U}(t)$	$P_3 Q_3 \mathbf{z}_3(t)$ $= c_3 \mathbf{U}(t)$
5	$\mathbf{Z}(t) = \mathbf{z}_1(t) + \mathbf{z}_2(t) + \mathbf{z}_3(t)$		
6 Solve	$F_1 G_1 \mathbf{y}_1(t)$ $= c_1 \mathbf{Z}(t)$	$F_2 G_2 \mathbf{y}_2(t)$ $= c_2 \mathbf{Z}(t)$	$F_3 G_3 \mathbf{y}_3(t)$ $= c_3 \mathbf{Z}(t)$
7	$\mathbf{Y}(t) = \mathbf{y}_1(t) + \mathbf{y}_2(t) + \mathbf{y}_3(t)$		
8 Solve	$L_1 U_1 \mathbf{w}_1(t)$ $= c_1 \mathbf{Y}(t)$	$L_2 U_2 \mathbf{w}_2(t)$ $= c_2 \mathbf{Y}(t)$	$L_3 U_3 \mathbf{w}_3(t)$ $= c_3 \mathbf{Y}(t)$
9	$\mathbf{U}(t+l) = \mathbf{w}_1(t) + \mathbf{w}_2(t) + \mathbf{w}_3(t)$		
10	GO TO Step 4 for next time step		

Table 2.5: Maximum errors for Example 1 at $t = 1.0$

Maximum analytical solution=0.10798D+00 (at the centre of the region).

N	7	9	19	39
h	0.25	0.2	0.1	0.05
l=0.125	0.22851D-3	0.19216D-3	0.17176D-3	0.17249D-3
Positions	2	3	9	20
l=0.1	0.17076D-3	0.12612D-3	0.91158D-4	0.90882D-4
Positions	2	3	9	20
l=0.05	0.11493D-3	0.69143D-4	0.17341D-4	0.12198D-4
Positions	2	2	6	18
l=0.025	-0.10762D-3	-0.68129D-4	0.95942D-5	0.22787D-5
Positions	6	7	5	12
l=0.0125	-0.10858D-3	-0.69231D-4	-0.10169D-4	0.12707D-5
Positions	6	7	15	9
l=0.01	-0.10865D-3	-0.69309D-4	-0.10238D-5	0.12078D-5
Positions	6	7	15	9
l=0.005	-0.10871D-3	-0.69381D-4	-0.10301D-5	-0.12570D-5
Positions	6	7	15	31
l=0.001	-0.10872D-3	-0.69390D-4	-0.10309D-5	-0.11422D-5
Positions	6	7	15	9

continued

Table 2.6: Continuation of Table 2.5

N	79	99	199	1999
h	0.025	0.02	0.01	0.001
l=0.125	0.17258D-3	0.17258D-3	0.17258D-3	0.17259D-3
Positions	40	50	100	999-1001
l=0.1	0.90972D-4	0.90976D-4	0.90978D-4	0.90995D-4
Positions	40	50	100	999-1001
l=0.05	0.12105D-4	0.12107D-4	0.12109D-4	0.12125D-4
Positions	39	50	100	995-1005
l=0.025	0.15822D-5	0.15694D-5	0.15658D-5	0.15813D-5
Positions	36	47	99	995-1005
l=0.0125	0.29266D-6	0.23299D-6	0.19977D-6	0.21439D-6
Positions	24	35	95	996-1004
l=0.01	0.21781D-6	0.15071D-6	0.10372D-6	0.10989D-6
Positions	21	30	90	999-1005
l=0.005	0.15522D-6	0.84170D-7	0.19206D-7	0.26640D-7
Positions	18	23	60	1012-1019
l=0.001	0.14761D-6	0.76423D-7	0.10387D-7	-0.96754D-8
Positions	18	22	47	997,999

Positions are shown by space steps.

Table 2.7: Maximum errors for Example 2 at the time t=1.0

Maximum analytical solution=0.91570D-02 (at the centre of the region).

N	7	9	19	39
h	0.25	0.2	0.1	0.05
l=0.125 Positions*	0.23709D-4 (3,3)	0.23909D-4 (4,4)	0.28442D-4 (10,10)	0.29197D-4 (20,20)
l=0.1 Positions	0.14754D-4 (2,2)	0.12703D-4 (3,3)	0.14702D-4 (9,9)	0.15371D-4 (20,20)
l=0.05 Positions	-0.22885D-4 (5,5)	-0.12926D-4 (7,7)	0.20732D-5 (7,7)	0.20168D-5 (19,19)
l=0.025 Positions	-0.24381D-4 (5,5)	-0.14285D-4 (6,7)	-0.15407D-5 (14,14)	0.30554D-6 (14,14)
l=0.02 Positions	-0.24490D-4 (5,5)	-0.14384D-4 (6,7)	-0.16279D-5 (13,14)	0.20717D-6 (13,13)
l=0.0125 Positions	-0.24578D-4 (5,5)	-0.14463D-4 (6,7)	-0.17023D-5 (13,14)	-0.16320D-6 (28,28)
l=0.01 Positions	-0.24592D-4 (5,5)	-0.14476D-4 (6,7)	-0.17141D-5 (13,14)	-0.17395D-6 (28,28)
l=0.005 Positions	-0.24605D-4 (5,5)	-0.14488D-4 (6,7)	-0.17250D-5 (13,14)	-0.18392D-6 (27,28)
l=0.001 Positions	-0.24607D-4 (5,5)	-0.14489D-4 (6,7)	-0.17265D-5 (13,14)	-0.18528D-6 (27,28)

continued

Table 2.8: Continuation of Table 2.7

N	49	79	99	199
h	0.04	0.025	0.02	0.01
l=0.125 Positions	0.29228D-4 (25,25)	0.29247D-4 (40,40)	0.29249D-4 (50,50)	0.29250D-4 (100,100)
l=0.1 Positions	0.15402D-4 (25,25)	0.15421D-4 (40,40)	0.15423D-4 (50,50)	0.15424D-4 (100,100)
l=0.05 Positions	0.20356D-5 (24,24)	0.20504D-5 (38,38)	0.20524D-5 (49,49)	0.20537D-5 (100,100)
l=0.025 Positions	0.27371D-6 (20,20)	0.26421D-6 (38,38)	0.26470D-6 (49,49)	0.26550D-6 (100,100)
l=0.02 Positions	0.16172D-6 (18,18)	0.13734D-6 (36,36)	0.13657D-6 (47,47)	0.13687D-6 (99,99) (99,100) (100,99)
l=0.0125 Positions	0.84932D-7 (15,15)	0.41439D-7 (29,29)	0.36021D-7 (41,41)	0.33663D-7 (97,97)
l=0.01 Positions	-0.80102D-7 (35,35)	0.28516D-7 (26,26)	0.21555D-7 (36,36)	0.17417D-7 (95,95)
l=0.005 Positions	-0.90020D-7 (35,35)	-0.19593D-7 (56,57)	0.10213D-7 (30,30)	0.28084D-8 (74,73) (74,74)
l=0.001 Positions	-0.91308D-7 (35,35)	-0.20892D-7 (56,56)	-0.10397D-7 (70,70)	-0.12919D-8 (60,59)

Positions are shown by space steps.

Table 2.9: Maximum errors for Example 3 at the time t=0.1

Maximum analytical solution=0.44701D+00 (at the centre of the region).

N	7	9	19	39
h	0.25	0.2	0.1	0.05
l=0.0125 Positions	-0.66171D-3 (5,5,5)	-0.35416D-3 (6,6,7) (6,7,6) (7,6,6)	-0.44384D-4 (13,13,13)	-0.50757D-5 (27,27,27)
l=0.01 Positions	-0.66180D-3 (5,5,5)	-0.35425D-3 (6,6,7) (6,7,6) (7,6,6)	-0.44474D-4 (13,13,13)	-0.51553D-5 (27,27,27)
l=0.005 Positions	-0.66189D-3 (5,5,5)	-0.35433D-3 (6,6,7) (6,7,6) (7,6,6)	-0.44557D-4 (13,13,13)	-0.52285D-5 (27,27,27)
l=0.001 Positions	-0.66190D-3 (5,5,5)	-0.35434D-3 (6,6,7) (6,7,6) (7,6,6)	-0.44568D-4 (13,13,13)	-0.52374D-5 (27,27,27)
l=0.0001 Positions	-0.66190D-3 (5,5,5)	-0.35434D-3 (6,6,7) (6,7,6) (7,6,6)	-0.44567D-4 (13,13,13)	-0.52373D-5 (27,27,27)

* Positions are shown by space steps.

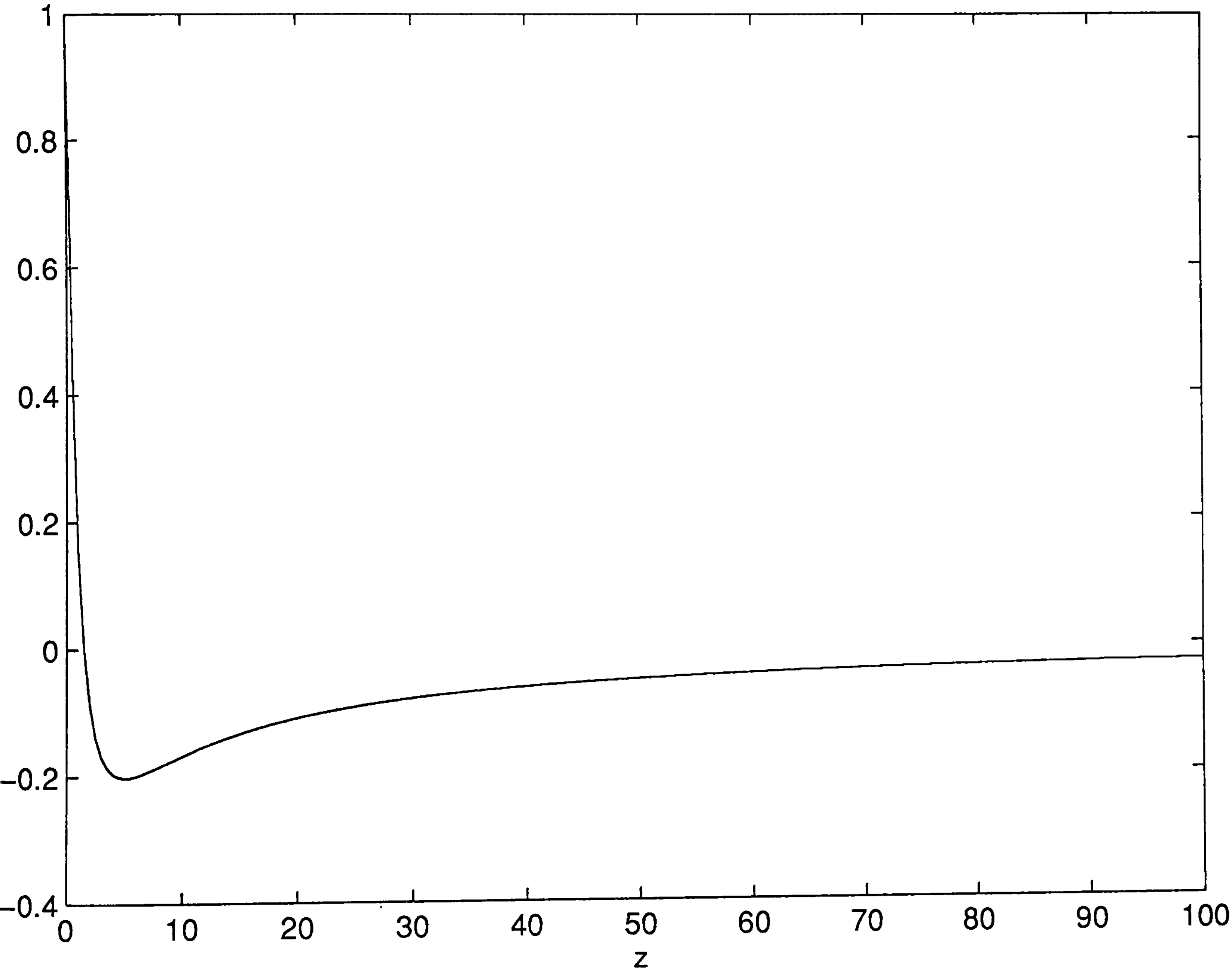

Figure 2.1: Graph of amplification symbol for third-order method.

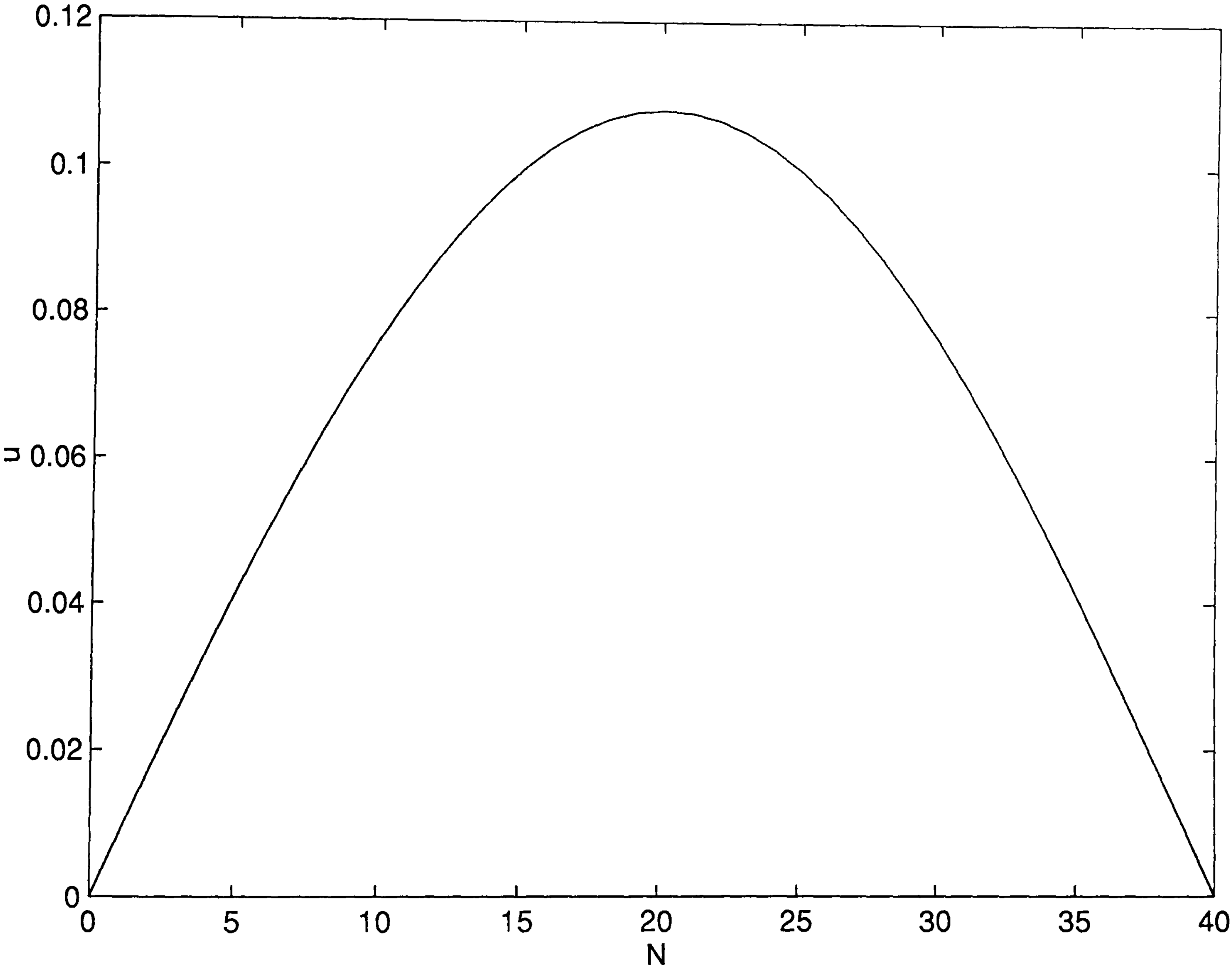

Figure 2.2: Theoretical solution of one dimensional heat equation at time t=1.

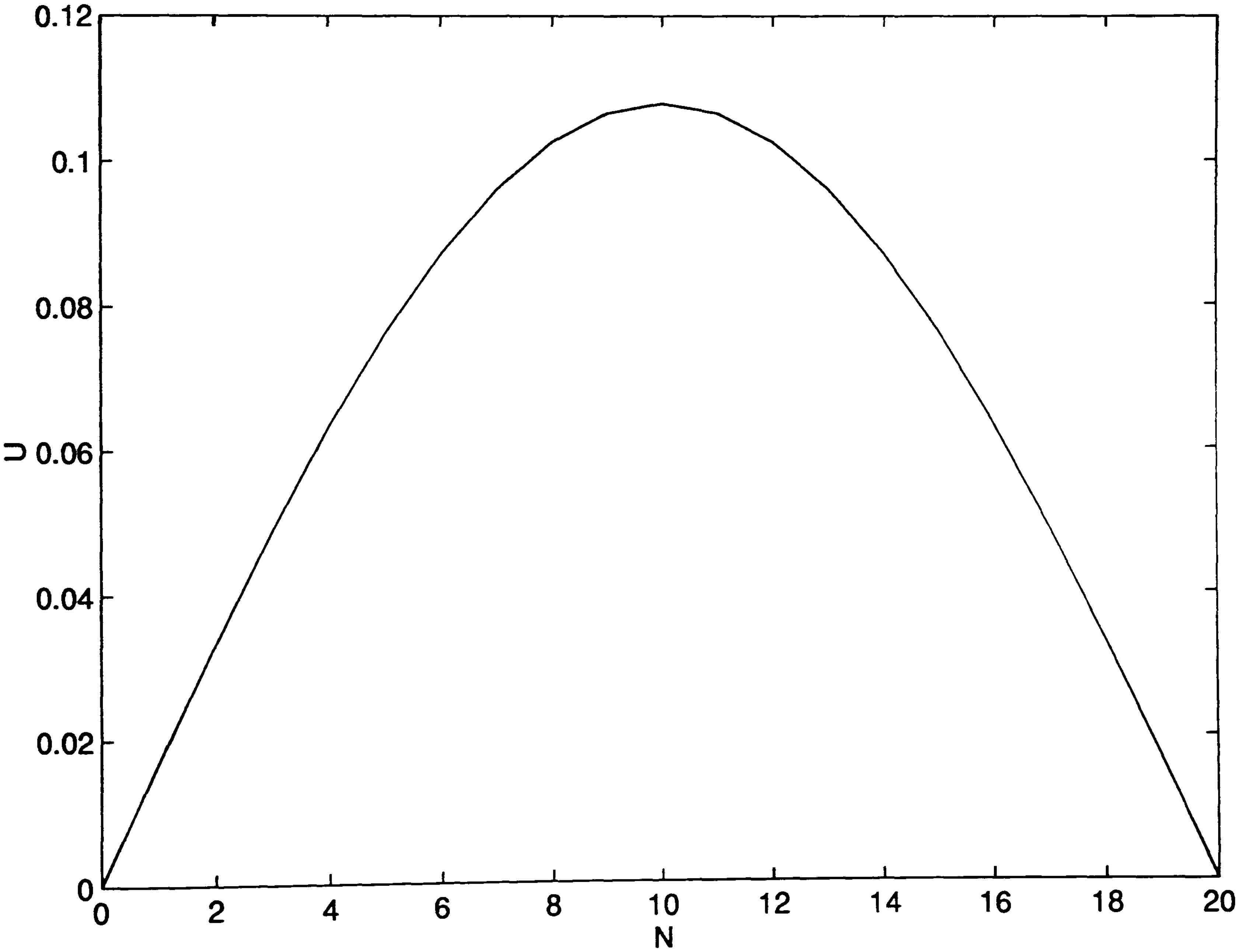

Figure 2.3: Numerical solution of one dimensional heat equation when $h=0.1$ and $l=0.1$ at time $t=1$.

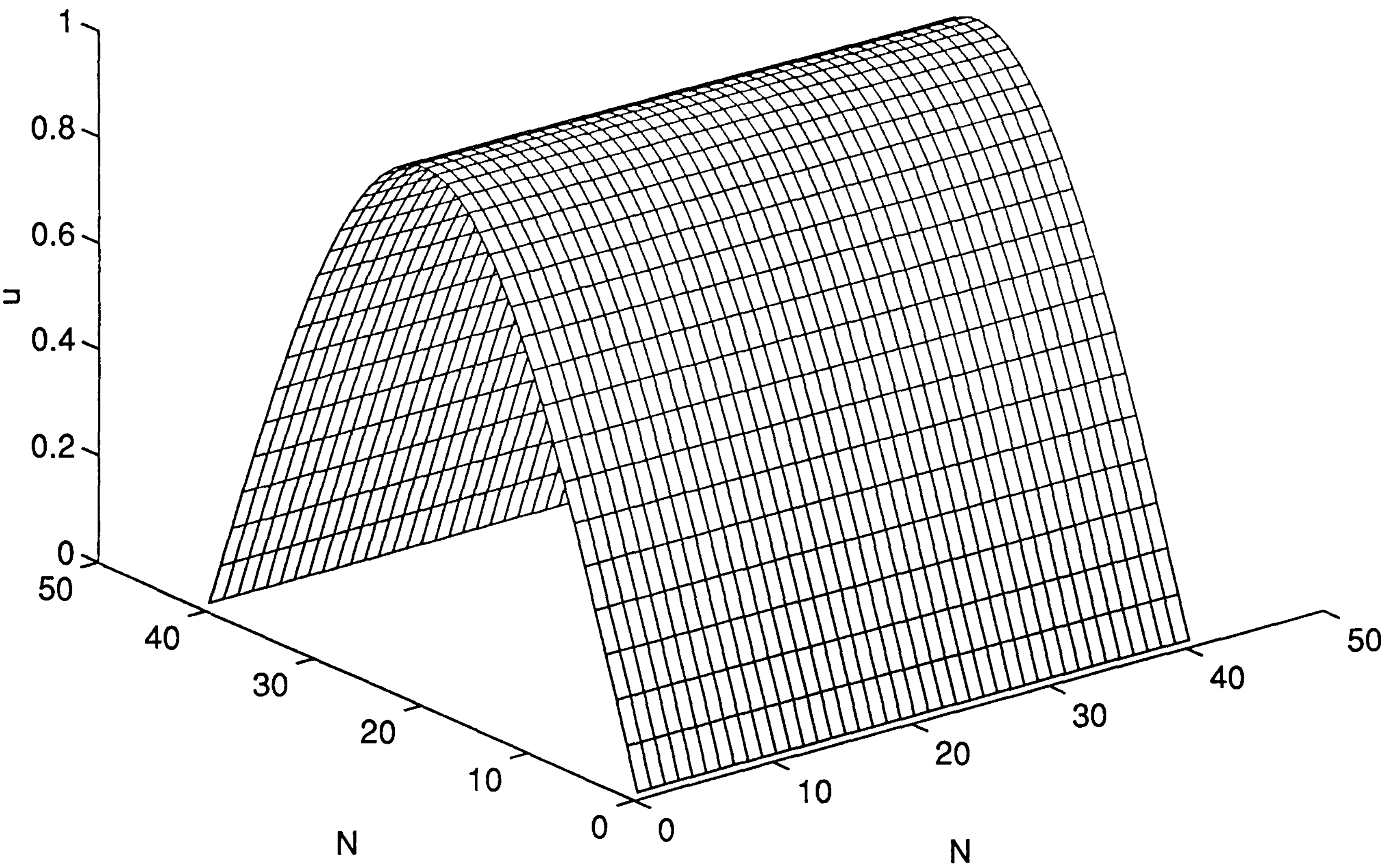

Figure 2.4: Initial distribution for two dimensional heat equation.

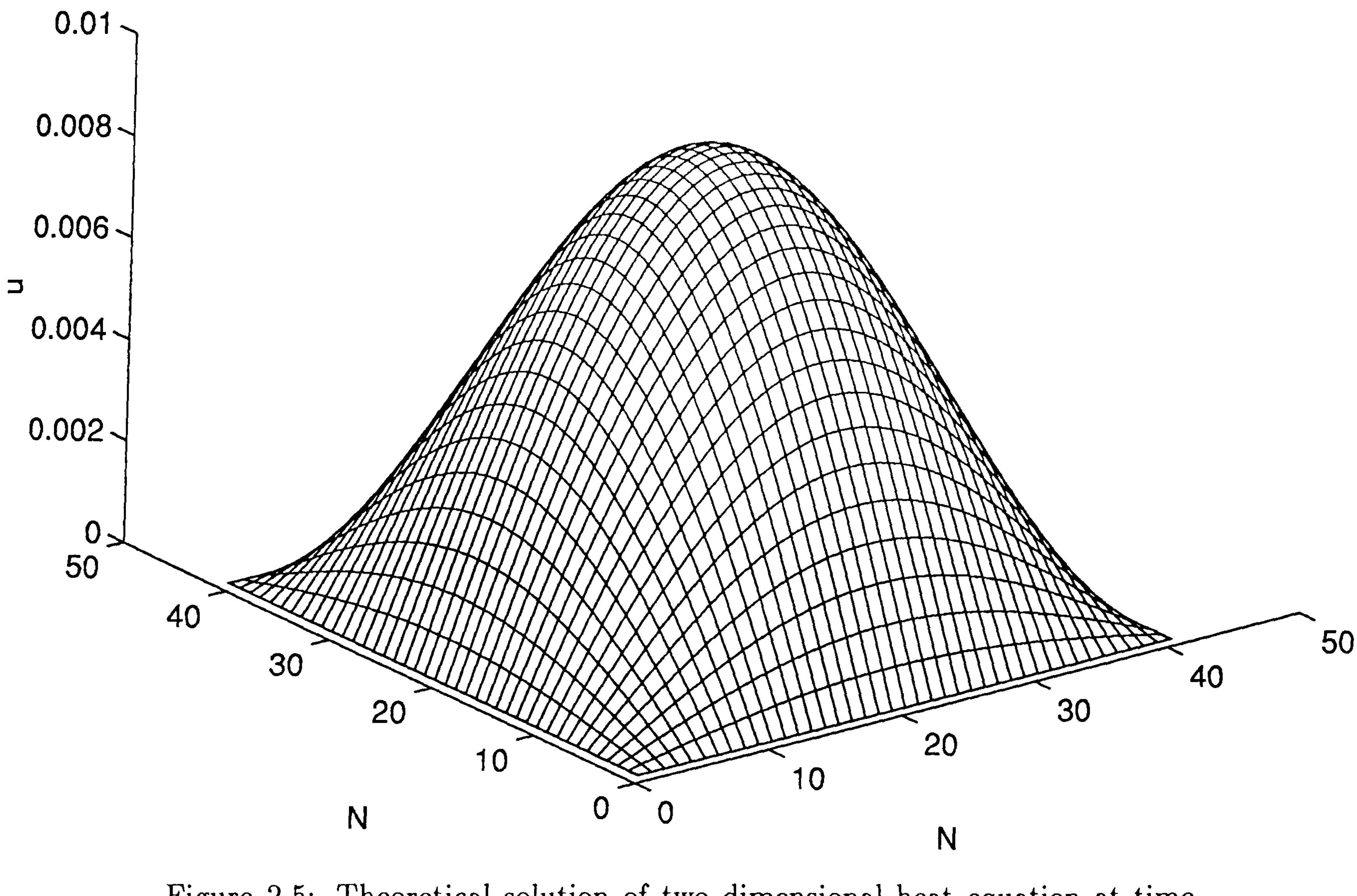

Figure 2.5: Theoretical solution of two dimensional heat equation at time t=1.

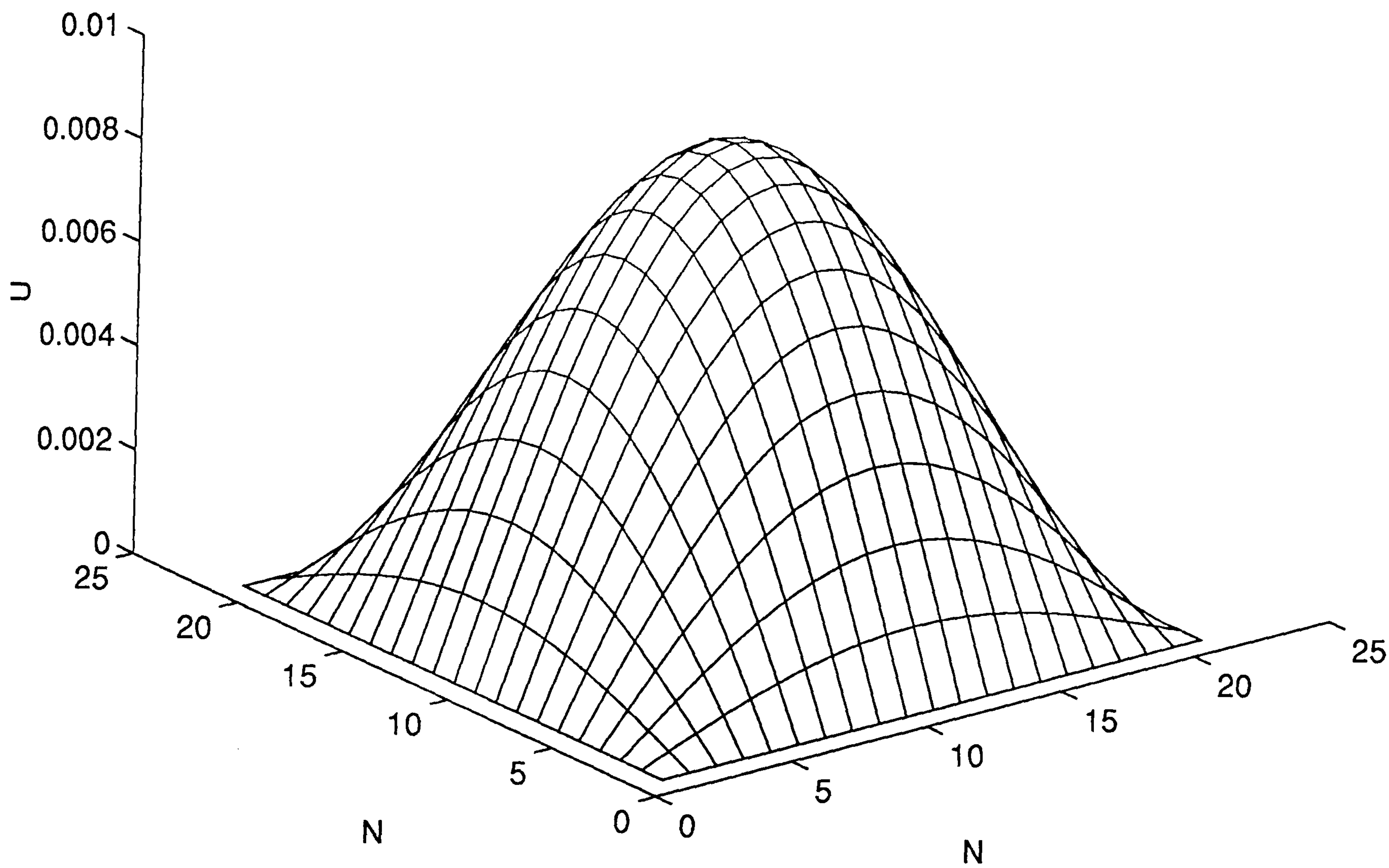

Figure 2.6: Numerical solution of two dimensional heat equation when h=0.1 and l=0.1 at t=1.

Chapter 3

Fourth-Order Numerical Methods

3.1 Derivation of the methods

For simplicity, consider the constant coefficient heat equation in one space variable{(2.1)–(2.3)} again:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad 0 < x < X, \quad t > 0 \qquad (3.1)$$

subject to the initial condition

$$u(x,0) = g(x), \quad 0 \leq x \leq X \qquad (3.2)$$

where $g(x)$ is a given continuous function of x, and the boundary conditions

$$u(0,t) = 0, \quad t > 0 \qquad (3.3)$$

$$u(X,t) = 0, \quad t > 0. \qquad (3.4)$$

There may exist discontinuities between initial and boundary conditions.

Divide the interval $[0, X]$ into $N + 1$ subintervals and then superimpose the region $[0 \leq x \leq X] \times [t \geq 0]$ by the rectangular mesh of points, with coordinates $(x_m, t_n) = (mh, nl)$ where $m = 0, 1, 2, \ldots, N+1, \quad n = 0, 1, 2, \ldots,$ $h(= \frac{X}{N+1})$ and l being step sizes in the $x-$ and $t-$directions respectively. To approximate the space derivative in (3.1) to fourth-order accuracy at some general point (x, t) of the mesh, assume that it may be replaced by the five-point formula

$$\begin{aligned} \frac{\partial^2 u(x,t)}{\partial x^2} &= \frac{1}{h^2}\{a\,u(x-2h,t) + b\,u(x-h,t) + c\,u(x,t) \\ &+ d\,u(x+h,t) + e\,u(x+2h,t)\}. \end{aligned} \quad (3.5)$$

Expanding the terms $u(x-2h,t)$, $u(x-h,t)$, $u(x+h,t)$ and $u(x+2h,t)$ in (3.5) about (x,t) gives

$$\begin{aligned} h^2\frac{\partial^2 u(x,t)}{\partial x^2} &= (a+b+c+d+e)\,u(x,t) \\ &+ (-2a-b+d+2e)\,h\frac{\partial u(x,t)}{\partial x} \\ &+ \frac{1}{2!}(4a+b+d+4e)\,h^2\frac{\partial^2 u(x,t)}{\partial x^2} \\ &+ \frac{1}{3!}(-8a-b+d+8e)\,h^3\frac{\partial^3 u(x,t)}{\partial x^3} \\ &+ \frac{1}{4!}(16a+b+d+16e)\,h^4\frac{\partial^4 u(x,t)}{\partial x^4} \\ &+ \frac{1}{5!}(-32a-b+d+32e)\,h^5\frac{\partial^5 u(x,t)}{\partial x^5} \\ &+ \frac{1}{6!}(64a+b+d+64e)\,h^6\frac{\partial^6 u(x,t)}{\partial x^6} \\ &+ \ldots \end{aligned} \quad (3.6)$$

Equating powers of $h^i (i = 0, 1, 2, 3, 4, 5)$ in (3.6) gives

$$\begin{aligned} a+b+c+d+e &= 0, \\ -2a-b+d+2e &= 0, \\ 4a+b+d+4e &= 2, \\ -8a-b+d+8e &= 0, \end{aligned} \quad (3.7)$$

$$
\begin{aligned}
16a + b + d + 16e &= 0, \\
-32a - b + d + 32e &= 0.
\end{aligned}
$$

A solution of the linear system (3.7) is

$$a = \frac{-1}{12}, \quad b = \frac{4}{3}, \quad c = \frac{-5}{2}, \quad d = \frac{4}{3}, \quad e = \frac{-1}{12} \qquad (3.8)$$

so that

$$
\begin{aligned}
\frac{\partial^2 u(x,t)}{\partial x^2} &= \frac{1}{12h^2}\{-u(x-2h,t) + 16\,u(x-h,t) - 30\,u(x,t) \\
&+ 16\,u(x+h,t) - \,u(x+2h,t)\} + \frac{1}{90}h^4\frac{\partial^6 u(x,t)}{\partial x^6} \\
&+ O(h^6)\, as \;\; h \to 0 \qquad (3.9)
\end{aligned}
$$

is a fourth-order approximation to the second-order space derivative at (x,t).

Equation (3.9) is valid only for $(x,t) = (x_m, t_n)$ with $m = 2, 3, \ldots, N-1$. To attain the same accuracy at the end points(x_1, t_n) and (x_N, t_n), special formulae must be developed which approximate $\partial^2 u(x,t)/\partial x^2$ not only to fourth order but also with dominant error term $\frac{1}{90}h^4\partial^6 u(x,t)/\partial x^6$ for $x = x_1, x_N$ and $t = t_n$. To achieve both of these, seven-point formulae will be needed in each case. It will also be useful to have the factor $(12h^2)^{-1}$ as in (3.9), as may be seen in (3.14) below.

Consider, then, the approximation to $\partial^2 u(x,t)/\partial x^2$ at the point $(x,t) = (x_1, t_n)$. Let

$$
\begin{aligned}
12\,h^2\frac{\partial^2 u(x,t)}{\partial x^2} &= a\,u(x-h,t) + b\,u(x,t) + c\,u(x+h,t) \\
&+ d\,u(x+2h,t) + e\,u(x+3h,t) + f\,u(x+4h,t) \\
&+ g\,u(x+5h,t) + \frac{2}{15}h^6\frac{\partial^6 u(x,t)}{\partial x^6}. \qquad (3.10)
\end{aligned}
$$

Then

$$12h^2\frac{\partial^2 u(x,t)}{\partial x^2} = (a+b+c+d+e+f+g)\,u(x,t)$$

$$
\begin{aligned}
&+ \quad (-a+c+2d+3e+4f+5g)\, h \frac{\partial u(x,t)}{\partial x} \\
&+ \quad \frac{1}{2!}(a+c+4d+9e+16f+25g)\, h^2 \frac{\partial^2 u(x,t)}{\partial x^2} \\
&+ \quad \frac{1}{3!}(-a+c+8d+27e+64f+125g)\, h^3 \frac{\partial^3 u(x,t)}{\partial x^3} \\
&+ \quad \frac{1}{4!}(a+c+16d+81e+256f+625g)\, h^4 \frac{\partial^4 u(x,t)}{\partial x^4} \\
&+ \quad \frac{1}{5!}(-a+c+32d+243e+1024f+3125g)\, h^5 \frac{\partial^5 u(x,t)}{\partial x^5} \\
&+ \quad \frac{1}{6!}(a+c+64d+729e+4096f+15625g)\, h^6 \frac{\partial^6 u(x,t)}{\partial x^6} \\
&+ \quad \frac{2}{15} h^6 \frac{\partial^6 u(x,t)}{\partial x^6} + \ldots \qquad (3.11)
\end{aligned}
$$

Equating powers of $h^i (i = 0, 1, 2, 3, 4, 5, 6)$ in (3.11) gives

$$
\begin{aligned}
a+b+c+d+e+f+g &= 0, \\
-a+c+2d+3e+4f+5g &= 0, \\
a+c+4d+9e+16f+25g &= 24, \\
-a+c+8d+27e+64f+125g &= 0, \qquad (3.12) \\
a+c+16d+81e+256f+625g &= 0, \\
-a+c+32d+243e+1024f+3125g &= 0, \\
a+c+64d+729e+4096f+15625g &= -96.
\end{aligned}
$$

The solution of the linear system (3.12) is

$$
\boxed{\begin{array}{llll} a = 9 & b = -9 & c = -19 & d = 34 \\ e = -21 & f = 7 & g = -1 & \end{array}} \qquad (3.13)
$$

so that, at the mesh point (x_1, t_n), the desired approximation to $\frac{\partial^2 u(x,t)}{\partial x^2}$ is

$$
\begin{aligned}
\frac{\partial^2 u(x,t)}{\partial x^2} &= \frac{1}{12h^2} \{9\, u(x-h,t) - 9\, u(x,t) - 19\, u(x+h,t) \\
&+ \quad 34\, u(x+2h,t) - 21\, u(x+3h,t) + 7\, u(x+4h,t) \\
&- \quad u(x+5h,t)\} + \frac{1}{90} h^4 \frac{\partial^6 u(x,t)}{\partial x^6} \\
&+ \quad O(h^5)\, as \quad h \to 0. \qquad (3.14)
\end{aligned}
$$

Suppose, now, that at the point $(x,t) = (x_N, t_n)$ the approximation to the second-order space derivative $\partial^2 u(x,t)/\partial x^2$ is given by

$$\begin{aligned} 12\,h^2 \frac{\partial^2 u(x,t)}{\partial x^2} &= a\,u(x-5h,t) + b\,u(x-4h,t) + c\,u(x-3h,t) \\ &+ d\,u(x-2h,t) + e\,u(x-h+h,t) + f\,u(x,t) \\ &+ g\,u(x+h,t) + \frac{2}{15} h^6 \frac{\partial^6 u(x,t)}{\partial x^6}. \end{aligned} \quad (3.15)$$

Then from (3.14) the values of the parameters, because of symmetry, are

$$\boxed{\begin{array}{llll} a=-1 & b=7 & c=-21 & d=34 \\ e=-19 & f=-9 & g=9 & \end{array}} \quad (3.16)$$

Hence, at the mesh point (x_N, t_n), the approximation to $\partial^2 u(x,t)/\partial x^2$ is

$$\begin{aligned} \frac{\partial^2 u(x,t)}{\partial x^2} &= \frac{1}{12h^2}\{-u(x-5h,t) + 7\,u(x-4h,t) - 21\,u(x-3h,t) \\ &+ 34\,u(x-2h,t) - 19\,u(x-h,t) - 9\,u(x,t) + 9\,u(x+h,t)\} \\ &+ \frac{1}{90} h^4 \frac{\partial^6 u(x,t)}{\partial x^6} + O(h^5)\; as \;\; h \to 0. \end{aligned} \quad (3.17)$$

Applying (3.1) with (3.9), (3.14) and (3.17) to the mesh points of the grid at time level $t = t_n$ produces a system of ODE's of the form

$$\frac{d\mathbf{U}(t)}{dt} = A\mathbf{U}(t), \quad t > 0 \quad (3.18)$$

with initial distribution

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

in which $\mathbf{U}(t) = [U_1(t), U_2(t), \ldots, U_N(t)]^T$, $\mathbf{g} = [g(x_1), g(x_2), \ldots, g(x_N)]^T$, T denoting transpose and

$$A = \frac{1}{12h^2}\begin{bmatrix} -9 & -19 & 34 & -21 & 7 & -1 & & & \bigcirc \\ 16 & -30 & 16 & -1 & & & & & \\ -1 & 16 & -30 & 16 & -1 & & & & \\ & -1 & 16 & -30 & 16 & -1 & & & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & & \\ & & & & -1 & 16 & -30 & 16 & -1 \\ & & & & & -1 & 16 & -30 & 16 \\ \bigcirc & & & -1 & 7 & -21 & 34 & -19 & -9 \end{bmatrix}_{N\times N} \quad (3.20)$$

The matrix h^2A has distinct eigenvalues with negative real parts for N=7,9,19 and 39 which are given in Appendix D. Solving (3.18) subject to (3.19) gives the solution

$$\mathbf{U}(t) = exp(lA)\mathbf{U}(0) \qquad (3.21)$$

which satisfies the recurrence relation

$$\mathbf{U}(t+l) = exp(lA)\mathbf{U}(t), \quad t = 0, l, 2l, \ldots. \qquad (3.22)$$

3.2 Fourth-Order Rational Approximant to $exp(lA)$

For $M = 4$ (2.24) gives

$$E_4(\theta) = \frac{b_0 + b_1\theta + b_2\theta^2 + b_3\theta^3}{a_0 - a_1\theta + a_2\theta^2 - a_3\theta^3 + a_4\theta^4}. \qquad (3.23)$$

Let

$$p(\theta) = b_0 + b_1\theta + b_2\theta^2 + b_3\theta^3 \qquad (3.24)$$

in which

$$\begin{aligned} b_0 &= 1, \\ b_1 &= 1 - a_1, \\ b_2 &= \tfrac{1}{2} - a_1 + a_2, \\ b_3 &= \tfrac{1}{6} - \tfrac{a_1}{2} + a_2 - a_3, \end{aligned}$$

and

$$q(\theta) = a_0 - a_1\theta + a_2\theta^2 - a_3\theta^3 + a_4\theta^4 \qquad (3.25)$$

where

$$a_4 = -\frac{1}{24} + \frac{a_1}{6} - \frac{a_2}{2} + a_3.$$

By (2.27)

$$\mu_4 = -\frac{1}{30} + \frac{a_1}{8} - \frac{a_2}{3} + \frac{a_3}{2}. \qquad (3.26)$$

3.3 L-Stability

Let λ be an eigenvalue of the matrix A given by (3.20). Then the amplification symbol of the numerical method arising from (3.23) is (Twizell (1984))

$$R(-z) = \frac{\sum_{k=0}^{3} a_k z^k - \sum_{k=1}^{3}[a_k - (-1)^k b_k] z^k}{\sum_{k=0}^{4} a_k z^k} \qquad (3.\ 27)$$

where $z = -lRe(\lambda) > 0$. Thus $L-$stability is guaranteed (Twizell (1984)) provided

$$a_4 > 0 \qquad (3.\ 28)$$

and

$$a_k - (-1)^k b_k \geq 0, \quad for\ all \quad k = 1, 2, 3 \qquad (3.\ 29)$$

or

$$(-1)^{k-1} \sum_{i=0}^{k-1} (-1)^i \frac{a_i}{(k-i)!} \geq 0, \quad for\ all\ k = 2, 3, 4. \qquad (3.\ 30)$$

So, for $M = 4$, L-stability is guaranteed provided together with (3.28)

$$a_1 > \frac{1}{2}, \qquad (3.\ 31)$$

$$a_2 > \frac{a_1}{2} - \frac{1}{6} \qquad (3.\ 32)$$

and then

$$a_3 > \frac{a_2}{2} - \frac{a_1}{6} + \frac{1}{24}. \qquad (3.\ 33)$$

3.4 Algorithm 1

Suppose that $r_i (i = 1, 2, 3, 4)$ are distinct real zeros of $q(\theta)$ defined by (3.25) then

$$exp(lA) = \sum_{i=1}^{4} c_i \left(I - \frac{l}{r_i} A \right)^{-1} \qquad (3.\ 34)$$

where the c_i ($i = 1,2,3,4$), the partial-fraction coefficients of $E_4(\theta)$, are defined by

$$c_i = \frac{p(r_i)}{\prod_{\substack{j=1 \\ j \neq i}}^{4} \left(1 - \frac{r_i}{r_j}\right)}, \quad i = 1,2,3,4 \tag{3.35}$$

So, using (3.34) in (3.22) gives

$$\mathbf{U}(t+l) = \left(\sum_{i=1}^{4} c_i \left(I - \frac{l}{r_i}A\right)^{-1}\right)\mathbf{U}(t). \tag{3.36}$$

Let

$$c_i \left(I - \frac{l}{r_i}A\right)^{-1} \mathbf{U}(t) = \mathbf{w}_i(t), \quad i = 1,2,3,4, \tag{3.37}$$

then

$$\left(I - \frac{l}{r_i}A\right)\mathbf{w}_i(t) = c_i\mathbf{U}(t), \quad i = 1,2,3,4 \tag{3.38}$$

and vector $\mathbf{w}_i(t)$ can be computed on processor i ($i = 1,2,3,4$). Consequently

$$\mathbf{U}(t+l) = \sum_{i=1}^{4} \mathbf{w}_i(t) \tag{3.39}$$

An algorithm, Algorithm 1, using four processors is detailed in Table 3.1.

3.5 Extension to two-space dimensions

Consider the two-dimensional heat equation with constant coefficients given by

$$\frac{\partial u(x,y,t)}{\partial t} = \frac{\partial^2 u(x,y,t)}{\partial x^2} + \frac{\partial^2 u(x,y,t)}{\partial y^2}, \quad 0 < x,y < X, \ t > 0 \tag{3.40}$$

subject to the initial conditions

$$u(x,y,0) = g(x,y), \quad 0 \leq x,y \leq X, \tag{3.41}$$

where $g(x,y)$ is a continuous function of x and y, and boundary conditions

$$u(0,y,t) = u(X,y,t) = 0, \quad t > 0 \tag{3.42}$$

$$u(x,0,t) = u(x,X,t) = 0, \quad t > 0 \tag{3.43}$$

Discretizing $0 \leq x, y \leq X$ as in the one-dimensional case and replacing the space derivatives in the PDE (3.40) by appropriate fourth-order difference approximations $\{(3.9), (3.14), (3.17)\}$ and applying to all N^2-interior mesh points at time level $t_n = nl; \quad n = 1, 2, 3, \ldots$, gives a system of N^2 first-order ordinary differential equations which may be written in matrix form as

$$\frac{d\mathbf{U}(t)}{dt} = A\mathbf{U}(t), \quad t > 0 \tag{3.44}$$

with

$$\mathbf{U}(0) = \mathbf{g}, \tag{3.45}$$

where $\mathbf{U}(t) = [U_{1,1}(t), U_{2,1}(t), \ldots, U_{N,1}(t), U_{1,2}(t), U_{2,2}(t), \ldots, U_{N,2}(t), \ldots, U_{1,N}(t), U_{2,N}(t), \ldots, U_{N,N}(t)]^T$ and $\mathbf{g} = [g_{1,1}, g_{2,1}, \ldots, g_{N,N}]^T$, T denoting transpose. The matrix A is the sum of two square matrices B and C of order N^2, given by

$$B = \frac{1}{12h^2}\begin{bmatrix} B_1 & & & \\ & B_1 & & \\ & & \ddots & \\ & & & B_1 \end{bmatrix} \tag{3.46}$$

where

$$B_1 = \begin{bmatrix} -9 & -19 & 34 & -21 & 7 & -1 & & \bigcirc \\ 16 & -30 & 16 & -1 & & & & \\ -1 & 16 & -30 & 16 & -1 & & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & & \\ & & -1 & 16 & -30 & 16 & -1 & \\ & & & -1 & 16 & -30 & 16 & -1 \\ & & & & -1 & 16 & -30 & 16 \\ \bigcirc & & -1 & 7 & -21 & 34 & -19 & -9 \end{bmatrix} \tag{3.47}$$

and

$$
C = \frac{1}{12h^2} \begin{bmatrix} -9I & -19I & 34I & -21I & 7I & -I & & \bigcirc \\ 16I & -30I & 16I & -I & & & & \\ -I & 16I & -30I & 16I & -I & & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & & \\ & & -I & 16I & -30I & 16I & -I & \\ & & & -I & 16I & -30I & 16I & -I \\ & & & & -I & 16I & -30I & 16I \\ \bigcirc & & -I & 7I & -21I & 34I & -19I & -9I \end{bmatrix} \qquad (3.48)
$$

where I is the identity matrix of order N. Clearly B and C commute. Solving (3.44) subject to the initial condition (3.45) gives (3.22).

3.5.1 Algorithm 2

Since $A = B + C$, and B and C commute (3.22) becomes

$$
\mathbf{U}(t + l) = exp(lB)exp(lC)\mathbf{U}(t), \quad t = 0, l, 2l, \ldots, \qquad (3.49)
$$

to fourth order. Using (3.34) gives

$$
exp(lB) = \sum_{i=1}^{4} c_i \left(I - \frac{l}{r_i} B \right)^{-1} \qquad (3.50)
$$

and

$$
exp(lC) = \sum_{i=1}^{4} c_i \left(I - \frac{l}{r_i} C \right)^{-1}. \qquad (3.51)
$$

So, (3.51) becomes

$$
\mathbf{U}(t + l) = \left(\sum_{i=1}^{4} c_i \left(I - \frac{l}{r_i} B \right)^{-1} \right) \left(\sum_{i=1}^{4} c_i \left(I - \frac{l}{r_i} C \right)^{-1} \right) \mathbf{U}(t). \qquad (3.52)
$$

Let

$$
\mathbf{z}_i(t) = c_i \left(I - \frac{l}{r_i} C \right)^{-1} \mathbf{U}(t), \quad i = 1, 2, 3, 4 \qquad (3.53)
$$

then the systems

$$\left(I - \frac{l}{r_i}C\right) \mathbf{z}_i(t) = c_i\mathbf{U}(t), \quad i = 1,2,3,4 \qquad (3.54)$$

can be solved on four different processors simultaneously. Let

$$\mathbf{Z}(t) = \sum_{i=1}^{4} \mathbf{z}_i(t), \qquad (3.55)$$

then (3.54) has the form

$$\mathbf{U}(t+l) = \left(\sum_{i=1}^{4} c_i \left(I - \frac{l}{r_i}B\right)^{-1}\right) \mathbf{Z}(t) \qquad (3.56)$$

or

$$\mathbf{U}(t+l) = \sum_{i=1}^{4} \mathbf{w}_i(t) \qquad (3.57)$$

where $\mathbf{w}_i (i = 1,2,3,4)$, the solutions of the linear systems

$$\left(I - \frac{l}{r_i}B\right) \mathbf{w}_i(t) = c_i\mathbf{Z}(t), \quad i = 1,2,3,4 \qquad (3.58)$$

can be computed on four differet processors simultaneously. Here $\mathbf{z}_i, \mathbf{w}_i$ $(i = 1,2,3,4)$ are intermediate vectors of order N^2. This algorithm is given in Table 3.2.

3.6 Extension to three-space dimensions

Consider the partial differential equation

$$\frac{\partial u(x,y,z,t)}{\partial t} = \frac{\partial^2 u(x,y,z,t)}{\partial x^2} + \frac{\partial^2 u(x,y,z,t)}{\partial y^2} + \frac{\partial^2 u(x,y,z,t)}{\partial z^2}, \qquad (3.59)$$

in the region $0 < x,y,z < X, \; t > 0$ subject to the initial conditions

$$u(x,y,z,0) = g(x,y,z), \quad 0 \le x,y,z \le X, \qquad (3.60)$$

where $g(x,y,z)$ is a continuous function of the space variables, and boundary conditions

$$\begin{aligned} u(0,y,z,t) &= u(X,y,z,t) = 0, \quad 0 \leq y,z \leq X \quad t > 0 \\ u(x,0,z,t) &= u(x,X,z,t) = 0, \quad 0 \leq x,z \leq X \quad t > 0 \\ u(x,y,0,t) &= u(x,y,X,t) = 0, \quad 0 \leq x,y \leq X \quad t > 0 \end{aligned} \tag{3.61}$$

Discretizing $0 \leq x,y,z \leq X$ as in the one-dimensional case and replacing the space derivatives in the PDE (3.59) by appropriate fourth-order difference approximations {(3.9), (3.14), (3.17)} and applying to all the N^3 interior mesh points at time level $t_n = nl$ $(n = 1,2,3,\ldots)$ leads to a system of N^3 first-order ordinary differential equations written in matrix form as

$$\frac{d\mathbf{U}(t)}{dt} = A\mathbf{U}(t), \quad t > 0 \tag{3.62}$$

with

$$\mathbf{U}(0) = \mathbf{g}, \tag{3.63}$$

where

$$\mathbf{U}(t) = [U_{1,1,1}(t), U_{2,1,1}(t), \ldots, U_{N,1,1}(t), U_{1,2,1}(t), U_{2,2,1}(t), \ldots, U_{N,N,N}(t)]^T$$

and

$$\mathbf{g} = [g_{1,1,1}, g_{2,1,1}, \ldots, g_{N,1,1}, g_{1,2,1}, g_{2,2,1}, \ldots, g_{N,N,N}]^T$$

, T denoting transpose. The square matrix A of order N^3 may be written as

$$A = A_1 + A_2 + A_3 \tag{3.64}$$

where A_1, A_2 and A_3 result from the replacements of the space derivatives in (3.59) by fourth-order difference approximations {(3.9), (3.14), (3.17)}. These three matrices commute and are given by

$$A_1 = \frac{1}{12h^2} \begin{bmatrix} B_1 & & & \\ & B_1 & & \\ & & \ddots & \\ & & & B_1 \end{bmatrix}, \tag{3.65}$$

a block-diagonal matrix with N^2 diagonal blocks given by

$$B_1 = \begin{bmatrix} -9 & -19 & 34 & -21 & 7 & -1 & & & \bigcirc \\ 16 & -30 & 16 & -1 & & & & & \\ -1 & 16 & -30 & 16 & -1 & & & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & & & \\ & & -1 & 16 & -30 & 16 & -1 & & \\ & & & -1 & 16 & -30 & 16 & -1 & \\ & & & & -1 & 16 & -30 & 16 & \\ \bigcirc & & -1 & 7 & -21 & 34 & -19 & -9 & \end{bmatrix}_{N\times N}, \qquad (3.66)$$

$$A_2 = \frac{1}{12h^2}\begin{bmatrix} B_2 & & & \\ & B_2 & & \\ & & \ddots & \\ & & & B_2 \end{bmatrix} \qquad (3.67)$$

which is a block-diagonal matrix with N diagonal blocks given by

$$B_2 = \begin{bmatrix} -9I & -19I & 34I & -21I & 7I & -I & & & \bigcirc \\ 16I & -30I & 16I & -I & & & & & \\ -I & 16I & -30I & 16I & -I & & & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & & & \\ & & -I & 16I & -30I & 16I & -I & & \\ & & & -I & 16I & -30I & 16I & -I & \\ & & & & -I & 16I & -30I & 16I & \\ \bigcirc & & -I & 7I & -21I & 34I & -19I & -9I & \end{bmatrix}_{N^2\times N^2} \qquad (3.68)$$

in which I is the identity matrix of order N, and

$$A_3 = \frac{1}{12h^2}\begin{bmatrix} -9I^* & -19I^* & 34I^* & -21I^* & 7I^* & -I^* & & & \bigcirc \\ 16I^* & -30I^* & 16I^* & -I^* & & & & & \\ -I^* & 16I^* & -30I^* & 16I^* & -I^* & & & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & & & \\ & & -I^* & 16I^* & -30I^* & 16I^* & -I^* & & \\ & & & -I^* & 16I^* & -30I^* & 16I^* & -I^* & \\ & & & & -I^* & 16I^* & -30I^* & 16I^* & \\ \bigcirc & & -I^* & 7I^* & -21I^* & 34I^* & -19I^* & -9I^* & \end{bmatrix}_{N^3\times N^3} \qquad (3.69)$$

where I^* is the identity matrix of order N^2. Solving (3.62) subject to the initial condition (3.63) gives (3.22).

3.6.1 Algorithm 3

Replacing A by $A_1 + A_2 + A_3$ in (3.22) gives, since A_1, A_2 and A_3 commute,

$$\mathbf{U}(t+l) = exp(lA_1)exp(lA_2)exp(lA_3)\mathbf{U}(t), \quad t = 0, l, 2l, \ldots. \qquad (3.70)$$

Using (3.34) gives

$$exp(lA_1) = \sum_{i=1}^{4} c_i \left(I - \frac{l}{r_i}A_1\right)^{-1}, \qquad (3.71)$$

$$exp(lA_2) = \sum_{i=1}^{4} c_i \left(I - \frac{l}{r_i}A_2\right)^{-1}, \qquad (3.72)$$

and

$$exp(lA_3) = \sum_{i=1}^{4} c_i \left(I - \frac{l}{r_i}A_3\right)^{-1}. \qquad (3.73)$$

So (3.70) becomes

$$\mathbf{U}(t+l) = \sum_{i=1}^{4} c_i \left(I - \frac{l}{r_i}A_1\right)^{-1} \sum_{i=1}^{4} c_i \left(I - \frac{l}{r_i}A_2\right)^{-1} \sum_{i=1}^{4} c_i \left(I - \frac{l}{r_i}A_3\right)^{-1} \mathbf{U}(t). \qquad (3.74)$$

Let

$$\mathbf{z}_i(t) = c_i \left(I - \frac{l}{r_i}A_3\right)^{-1} \mathbf{U}(t), \quad i = 1, 2, 3, 4 \qquad (3.75)$$

then

$$\left(I - \frac{l}{r_i}A_3\right) \mathbf{z}_i(t) = c_i\mathbf{U}(t), \quad i = 1, 2, 3, 4. \qquad (3.76)$$

Taking

$$\mathbf{Z}(t) = \sum_{i=1}^{4} \mathbf{z}_i(t), \qquad (3.77)$$

leads to

$$\mathbf{U}(t+l) = \sum_{i=1}^{4} c_i \left(I - \frac{l}{r_i}A_1\right)^{-1} \sum_{i=1}^{4} c_i \left(I - \frac{l}{r_i}A_2\right)^{-1} \mathbf{Z}(t). \qquad (3.78)$$

Let

$$\mathbf{y}_i(t) = c_i \left(I - \frac{l}{r_i}A_2\right)^{-1} \mathbf{Z}(t), \quad i = 1, 2, 3, 4 \qquad (3.79)$$

then

$$\left(I - \frac{l}{r_i}A_2\right)\mathbf{y}_i(t) = c_i\mathbf{Z}(t), \quad i = 1,2,3,4. \tag{3.80}$$

Let

$$\mathbf{Y}(t) = \sum_{i=1}^{4}\mathbf{y}_i(t), \tag{3.81}$$

then (3.78) becomes

$$\mathbf{U}(t+l) = \sum_{i=1}^{4}\mathbf{w}_i(t), \tag{3.82}$$

where $\mathbf{w}_i; i = 1,2,3,4$, are the solutions of the linear systems

$$\left(I - \frac{l}{r_i}A_1\right)\mathbf{w}_i(t) = c_i\mathbf{Y}(t), \quad i = 1,2,3,4. \tag{3.83}$$

Here {(3.76),(3.77),(3.80)–(3.83)} constitute the algorithm. Using this algorithm four different processors can be used simultaneously thrice. Details of this algorithm, Algorithm 3, are given in Table 3.3.

3.7 Numerical Examples

In this section only a representative of the methods based on (3.23) will be used. Using

$$a_1 = \frac{64}{25}, a_2 = \frac{7}{3}, a_3 = \frac{547}{600}$$

in (3.23) through (3.25) gives

$$b_1 = -\frac{39}{25}, b_2 = \frac{41}{150}, b_3 = \frac{37}{120},$$

and

$$a_4 = \frac{13}{100},$$

and then it is found that

$$r_1 = 0.93758090808524, \quad r_2 = 1.8147198580060,$$

$$r_3 = 2.0000000000000, \quad r_4 = 2.2605197467293$$

are the real zeros of $q(\theta)$, given by (3.25). Using these values in (3.35) produces

$$c_1 = 0.21145556670851, \quad c_2 = -53.350306744604$$

$$c_3 = 108.00000000002, \quad c_4 = -53.861148822124.$$

Here values are only given to 14 significant figures. According to these values of the parameters amplification symbol is depicted in Figure 3.1. Some other values of the parameters are given in Appendix E.

3.7.1 One-dimensional Problem

Example 1

Considering the one space dimensional heat equation with constant coefficients (3.1) and taking $X = 2$ and $g(x) = 1$ in {(3.1)-(3.3)} the model problem {(2.92)-(2.94)} of Chapter 2 is used again: it is repeated here for convenience

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad 0 < x < 2, \quad t > 0 \tag{3. 84}$$

subject to the initial condition

$$u(x, 0) = 1, \quad 0 \leq x \leq 2 \tag{3. 85}$$

and boundary conditions

$$u(0, t) = u(2, t) = 0, \quad t > 0. \tag{3. 86}$$

This problem, which has theoretical solution

$$u(x, t) = \sum_{k=1}^{\infty} [1 - (-1)^k] \frac{2}{k\pi} sin(\frac{k\pi x}{2}) exp(-\frac{k^2\pi^2 t}{4}), \tag{3. 87}$$

(Lawson and Morris, 1978) has discontinuities between initial conditions and boundary conditions at $x = 0$ and $x = 2$. The theoretical solution at time $t = 1.0$ is depicted in Figure 2.2 of chapter 2.

Using Algorithm 1 the model problem {(3.84)–(3.86)} is solved for

$$h = 0.25, 0.2, 0.1, 0.05, 0.04, 0.025, 0.02, 0.01$$

using

$$l = 0.125, 0.1, 0.05, 0.025, 0.0125, 0.01, 0.005, 0.002, 0.001.$$

In these experiments the method behaves smoothly over the whole interval $0 \leq x \leq 2$ and gives maximum errors at the centre of the region except the cases which are starred in Table 3.4 which gives the maximum errors at the time $t = 1.0$.

It may be deduced from Table 3.4 that the optimal value of r $(= \frac{l}{h})$ for this problem lies in the interval [0.3, 0.32]. So selecting carefully the values of h and l the accuracy can be remarkably increased. For example , using $l = \frac{1}{20}$ and $h = \frac{1}{6}$ the maximum error obtained is $0.34052D - 07$ while for $l = \frac{1}{20}$ and $h = \frac{1}{5}$ the maximum error is $-0.20738D - 05$. Similarly for $l = \frac{1}{94}$ and $h = \frac{1}{30}$ the maximum error is $0.48468D - 10$, and for $l = \frac{1}{188}$ and $h = \frac{1}{60}$ the maximum error is $0.34070D - 11$. The numerical solution for $h = 0.1$ with $l = 0.1$ is depicted in Figure 3.2. All other numerical solutions give similar graphs.

3.7.2 Two-dimensional Problem

Example 2

Considering the two space dimensional heat equation with constant coefficients {(2.46)-(2.49)} with $X = 2$ and $g(x,y) = sin(\frac{\pi}{2}y)$ the model problem becomes

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}, \quad 0 < x, y < 2, \quad t > 0 \qquad (3.88)$$

subject to the initial condition

$$u(x,y,0) = sin(\frac{\pi y}{2}), \quad 0 \leq x, y \leq 2 \qquad (3.89)$$

and the boundary conditions

$$u(x,y,t) = 0, \quad t > 0 \qquad (3.90)$$

on the lines $x = 0$, $y = 0$, $x = 2$ and $y = 2$.

The initial distribution is shown in Figure 2.5 of Chapter 2 and the theoretical solution of this problem,

$$u(x,y,t) = sin(\frac{\pi}{2}y)\sum_{k=1}^{\infty}[1-(-1)^k]\frac{2}{k\pi}sin(\frac{k\pi x}{2})exp(-\frac{(k^2+1)\pi^2 t}{4}), \qquad (3.91)$$

(given by Lawson and Morris, 1978) is depicted at time $t = 1.0$ in Figure 2.5 of Chapter 2. The maximum value of u at time $t = 1.0$ occurs for $(x,y) = (1,1)$ and is approximately 0.00915699.

Since the initial function does not necessarily have the value zero on the square, for example, $u(0,1,0) = 1$, discontinuities between initial conditions and boundary conditions do exist.

Using Algorithm 2 the model problem {(3.88)–(3.90)} is solved for

$$l = 0.125, 0.1, 0.05, 0.025, 0.02, 0.0125, 0.01, 0.005, 0.001$$

using

$$h = 0.25, 0.2, 0.1, 0.05, 0.04, 0.025, 0.02, 0.01.$$

The numerical solution for $h = 0.1$ with $l = 0.1$ is depicted in Figure 3.3. All other numerical solutions produce similar graphs. In these experiments the method behaves smoothly over the whole interval $0 \leq x \leq 2$ and gives maximum error modulus at the centre of the region. Maximum errors at time $t = 1.0$ are given in Table 3.6.

It is calculated from Table 3.6 that the optimistic value of r $(= \frac{l}{h})$ for this problem lies in the interval [0.41, 0.43]. So, selecting carefully the values of h and l the accuracy can be remarkably increased. For example, using $l = 0.05$ and $h = \frac{1}{9}$ the maximum error obtained is $0.12824D - 07$ while for $l = 0.05$ and $h = \frac{1}{10}$ the maximum error is $0.11240D - 06$. Similarly for $l = 0.0125$ and $h = \frac{1}{34}$ the maximum error is $0.31464D - 11$, and for $l = 0.005$ and $h = \frac{1}{85}$ the maximum error is $0.17011D - 11$.

3.7.3 Three-dimensional Problem

Example 3

Considering the three space dimensional heat equation with constant coefficients {(3.59)-(3.61)} with $X = 2$ and $g(x, y, z) = sin(\frac{\pi}{2}x)sin(\frac{\pi}{2}y)sin(\frac{\pi}{2}z)$, the model problem becomes

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}, \quad 0 < x, y, z < 2, \quad t > 0 \qquad (3.92)$$

subject to the initial condition

$$u(x, y, z, 0) = sin(\frac{1}{2}\pi x)sin(\frac{1}{2}\pi y)sin(\frac{1}{2}\pi z), \quad 0 \leq x, y, z \leq 2 \qquad (3.93)$$

and the boundary conditions

$$u(x,y,z,t) = 0, \quad t > 0 \tag{3. 94}$$

on the planes $x = 0$, $y = 0$, $z = 0$, $x = 2$, $y = 2$ and $z = 2$.

The theoretical solution of this problem is

$$u(x,y,z,t) = sin(\frac{\pi}{2}x)sin(\frac{\pi}{2}y)sin(\frac{\pi}{2}z)exp(-\frac{3}{4}\pi^2 t). \tag{3. 95}$$

The maximum value of u at time $t = 0.1$ occurs for $(x,y,z) = (1,1,1)$ and is approximately 0.44701 .

Using Algorithm 3 the model problem {(3.92)–(3.94)} is solved for $l = 0.0125, 0.01, 0.005, 0.001, 0.0001$ using h=0.25, 0.2, 0.1, 0.05. In these experiments the method behaves smoothly over the whole interval $0 \leq x, y, z \leq 2$ and gives maximum error modulus at the centre of the region. Maximum errors at the time $t = 0.1$ are given in Table 3.8.

Table 3.1: 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 Solve	$L_1U_1\mathbf{w}_1(t)$ $= c_1\mathbf{U}(t)$	$L_2U_2\mathbf{w}_2(t)$ $= c_2\mathbf{U}(t)$	$L_3U_3\mathbf{w}_3(t)$ $= c_3\mathbf{U}(t)$	$L_4U_4\mathbf{w}_4(t)$ $= c_4\mathbf{U}(t)$
5	$\mathbf{U}(t+l) = \mathbf{w}_1(t) + \mathbf{w}_2(t) + \mathbf{w}_3(t) + \mathbf{w}_4(t)$			
6	GO TO Step 4 for next time step			

Table 3.2: Algorithm 2

Steps	Processor 1	Processor 2	Processor 3	Processor 4
1 Input	l, r_1, c_1 $\mathbf{U}_0, B, C$	l, r_2, c_2 $\mathbf{U}_0, B, C$	l, r_3, c_3 $\mathbf{U}_0, B, C$	l, r_4, c_4 $\mathbf{U}_0, B, C$
2 Compute	$I - \frac{l}{r_1}B$ $I - \frac{l}{r_1}C$	$I - \frac{l}{r_2}B$ $I - \frac{l}{r_2}C$	$I - \frac{l}{r_3}B$ $I - \frac{l}{r_3}C$	$I - \frac{l}{r_4}B$ $I - \frac{l}{r_4}C$
3 Decompose	$I - \frac{l}{r_1}B = L_1U_1$ $I - \frac{l}{r_1}C = P_1Q_1$	$I - \frac{l}{r_2}B = L_2U_2$ $I - \frac{l}{r_2}C = P_2Q_2$	$I - \frac{l}{r_3}B = L_3U_3$ $I - \frac{l}{r_3}C = P_3Q_3$	$I - \frac{l}{r_4}B = L_4U_4$ $I - \frac{l}{r_4}C = P_4Q_4$
4 Solve	$P_1Q_1\mathbf{z}_1(t) = c_1\mathbf{U}(t)$	$P_2Q_2\mathbf{z}_2(t) = c_2\mathbf{U}(t)$	$P_3Q_3\mathbf{z}_3(t) = c_3\mathbf{U}(t)$	$P_4Q_4\mathbf{z}_4(t) = c_4\mathbf{U}(t)$
5	$\mathbf{Z}(t) = \mathbf{z}_1(t) + \mathbf{z}_2(t) + \mathbf{z}_3(t) + \mathbf{z}_4(t)$			
6 Solve	$L_1U_1\mathbf{w}_1(t) = c_1\mathbf{Z}(t)$	$L_2U_2\mathbf{w}_2(t) = c_2\mathbf{Z}(t)$	$L_3U_3\mathbf{w}_3(t) = c_3\mathbf{Z}(t)$	$L_4U_4\mathbf{w}_4(t) = c_4\mathbf{Z}(t)$
7	$\mathbf{U}(t + l) = \mathbf{w}_1(t) + \mathbf{w}_2(t) + \mathbf{w}_3(t) + \mathbf{w}_4(t)$			
8	GO TO Step 4 for next time step			

Table 3.3: Algorithm 3

Steps	Processor 1	Processor 2	Processor 3	Processor 4
1 Input	$l, r_1, c_1, \mathbf{U}_0, A_1, A_2, A_3$	$l, r_2, c_2, \mathbf{U}_0, A_1, A_2, A_3$	$l, r_3, c_3, \mathbf{U}_0, A_1, A_2, A_3$	$l, r_4, c_4, \mathbf{U}_0, A_1, A_2, A_3$
2 Compute	$I - \frac{l}{r_1}A_1$ $I - \frac{l}{r_1}A_2$ $I - \frac{l}{r_1}A_3$	$I - \frac{l}{r_2}A_1$ $I - \frac{l}{r_2}A_2$ $I - \frac{l}{r_2}A_3$	$I - \frac{l}{r_3}A_1$ $I - \frac{l}{r_3}A_2$ $I - \frac{l}{r_3}A_3$	$I - \frac{l}{r_4}A_1$ $I - \frac{l}{r_4}A_2$ $I - \frac{l}{r_4}A_3$
3 Decompose	$I - \frac{l}{r_1}A_3 = P_1Q_1$ $I - \frac{l}{r_1}A_2 = F_1G_1$ $I - \frac{l}{r_1}A_1 = L_1U_1$	$I - \frac{l}{r_2}A_3 = P_2Q_2$ $I - \frac{l}{r_2}A_2 = F_2G_2$ $I - \frac{l}{r_2}A_1 = L_2U_2$	$I - \frac{l}{r_3}A_3 = P_3Q_3$ $I - \frac{l}{r_2}A_3 = F_3G_3$ $I - \frac{l}{r_3}A_1 = L_3U_3$	$I - \frac{l}{r_4}A_3 = P_4Q_4$ $I - \frac{l}{r_4}A_2 = F_4G_4$ $I - \frac{l}{r_4}A_1 = L_4U_4$
4 Solve	$P_1Q_1\mathbf{z}_1(t) = c_1\mathbf{U}(t)$	$P_2Q_2\mathbf{z}_2(t) = c_2\mathbf{U}(t)$	$P_3Q_3\mathbf{z}_3(t) = c_3\mathbf{U}(t)$	$P_4Q_4\mathbf{z}_4(t) = c_4\mathbf{U}(t)$
5	$\mathbf{Z}(t) = \mathbf{z}_1(t) + \mathbf{z}_2(t) + \mathbf{z}_3(t) + \mathbf{z}_4(t)$			
6 Solve	$F_1G_1\mathbf{y}_1(t) = c_1\mathbf{Z}(t)$	$F_2G_2\mathbf{y}_2(t) = c_2\mathbf{Z}(t)$	$F_3G_3\mathbf{y}_3(t) = c_3\mathbf{Z}(t)$	$F_4G_4\mathbf{y}_4(t) = c_4\mathbf{Z}(t)$
7	$\mathbf{Y}(t) = \mathbf{y}_1(t) + \mathbf{y}_2(t) + \mathbf{y}_3(t) + \mathbf{y}_4(t)$			
8 Solve	$L_1U_1\mathbf{w}_1(t) = c_1\mathbf{Y}(t)$	$L_2U_2\mathbf{w}_2(t) = c_2\mathbf{Y}(t)$	$L_3U_3\mathbf{w}_3(t) = c_3\mathbf{Y}(t)$	$L_4U_4\mathbf{w}_4(t) = c_4\mathbf{Y}(t)$
9	$\mathbf{U}(t+l) = \mathbf{w}_1(t) + \mathbf{w}_2(t) + \mathbf{w}_3(t) + \mathbf{w}_4(t)$			
10	GO TO Step 4 for next time step			

Table 3.4: Maximum errors for Example 1 at $t = 1.0$

Maximum analytical solution=0.10798D+00 (at the centre of the region).

N	7	9	19	39
h	0.25	0.2	0.1	0.05
l=0.125	0.49826D-4	0.49496D-4	0.51699D-4	0.51994D-4
l=0.1	0.21120D-4	0.20762D-4	0.22949D-4	0.23243D-4
l=0.05	-0.62417D-5⋆	-0.20738D-5*	0.14443D-5	0.17379D-5
l=0.025	-0.68672D-5⋆	-0.26782D-5*	-0.19279D-6	0.10078D-6
l=0.0125	-0.69107D-5⋆	-0.27451D-5*	-0.30667D-6	-0.13107D-7
l=0.01	-0.69125D-5⋆	-0.27479D-5*	-0.31138D-6	-0.17820D-7
l=0.005	-0.69137D-5⋆	-0.27497D-5*	-0.31450D-6	-0.20938D-7
l=0.002	-0.69138D-5⋆	-0.27498D-5*	-0.31471D-6	-0.21147D-7
l=0.001	-0.69138D-5⋆	-0.27498D-5*	-0.31472D-6	-0.21153D-7

⋆ indicates positions 1 and 7 and * positions 2 and 8

contined

Table 3.5: Continuation of Table 3.4

N	49	79	99	199
h	0.04	0.025	0.02	0.01
l=0.125	0.52007D-4	0.52014D-4	0.52015D-4	0.52015D-4
l=0.1	0.23256D-4	0.23263D-4	0.23264D-4	0.23264D-4
l=0.05	0.17503D-5	0.17577D-5	0.17585D-5	0.17590D-5
l=0.025	0.11323D-6	0.12060D-6	0.12139D-6	0.12191D-6
l=0.0125	-0.65816D-9	0.67127D-8	0.75003D-8	0.80192D-8
l=0.01	-0.53710D-8	0.19985D-8	0.27865D-8	0.33035D-8
l=0.005	-0.84894D-8	-0.11196D-8	-0.33055D-9	0.18801D-9
l=0.002	-0.86970D-8	-0.13318D-8	-0.53868D-9	-0.10847D-10
l=0.001	-0.87055D-8	-0.13403D-8	-0.54262D-9	-0.37895D-10

Table 3.6: Maximum errors for Example 2 at the time t=1.0

Maximum analytical solution=0.91570D-02 (at the centre of the region).

N	7	9	19	39
h	0.25	0.2	0.1	0.05
l=0.125	0.37425D-6	0.55378D-5	0.86345D-5	0.88091D-5
l=0.1	-0.44973D-5	0.66405D-6	0.37595D-5	0.39341D-5
l=0.05	-0.81415D-5	-0.29820D-5	0.11240D-6	0.28696D-6
l=0.025	-0.84189D-5	-0.32596D-5	-0.16527D-6	0.92834D-8
l=0.02	-0.84309D-5	-0.32716D-5	-0.17730D-6	-0.27429D-8
l=0.0125	-0.84382D-5	-0.32789D-5	-0.18459D-6	-0.10033D-7
l=0.01	-0.84390D-5	-0.32797D-5	-0.18538D-6	-0.10832D-7
l=0.005	-0.84395D-5	-0.32803D-5	-0.18591D-6	-0.11361D-7
l=0.001	-0.84396D-5	-0.32803D-5	-0.18595D-6	-0.11397D-7

continued

Table 3.7: Continuation of Table 3.6

N	49	79	99	199
h	0.04	0.025	0.02	0.01
l=0.125	0.88159D-5	0.88198D-5	0.88203D-5	0.88205D-5
l=0.1	0.39408D-5	0.39448D-5	0.39452D-5	0.39455D-5
l=0.05	0.29669D-6	0.29764D-6	0.29806D-6	0.29833D-6
l=0.025	0.16019D-7	0.19970D-7	0.20389D-7	0.20660D-7
l=0.02	0.39932D-8	0.79439D-8	0.83637D-8	0.86374D-8
l=0.0125	-0.32970D-8	0.65423D-9	0.10730D-8	0.13450D-8
l=0.01	-0.40961D-8	-0.14549D-9	0.27407D-9	0.54852D-9
l=0.005	-0.46252D-8	-0.67374D-9	-0.25487D-9	0.20241D-10
l=0.001	-0.46612D-8	-0.71152D-9	-0.29076D-9	-0.14262D-10

Table 3.8: Maximum errors for Example 3 at the time t=0.1

Maximum analytical solution=0.44701D+00 (at the centre of the region).

N	7	9	19	39
h	0.25	0.2	0.1	0.05
l=0.0125	-0.10186D-3	-0.40366D-4	-0.23963D-5	-0.13873D-6
l=0.01	-0.10186D-3	-0.40373D-4	-0.24025D-5	-0.14498D-6
l=0.005	-0.10187D-3	-0.40377D-4	-0.24067D-5	-0.14911D-6
l=0.001	-0.10187D-3	-0.40377D-4	-0.24070D-5	-0.14939D-6
l=0.0001	-0.10187D-3	-0.40377D-4	-0.24070D-5	-0.14943D-6

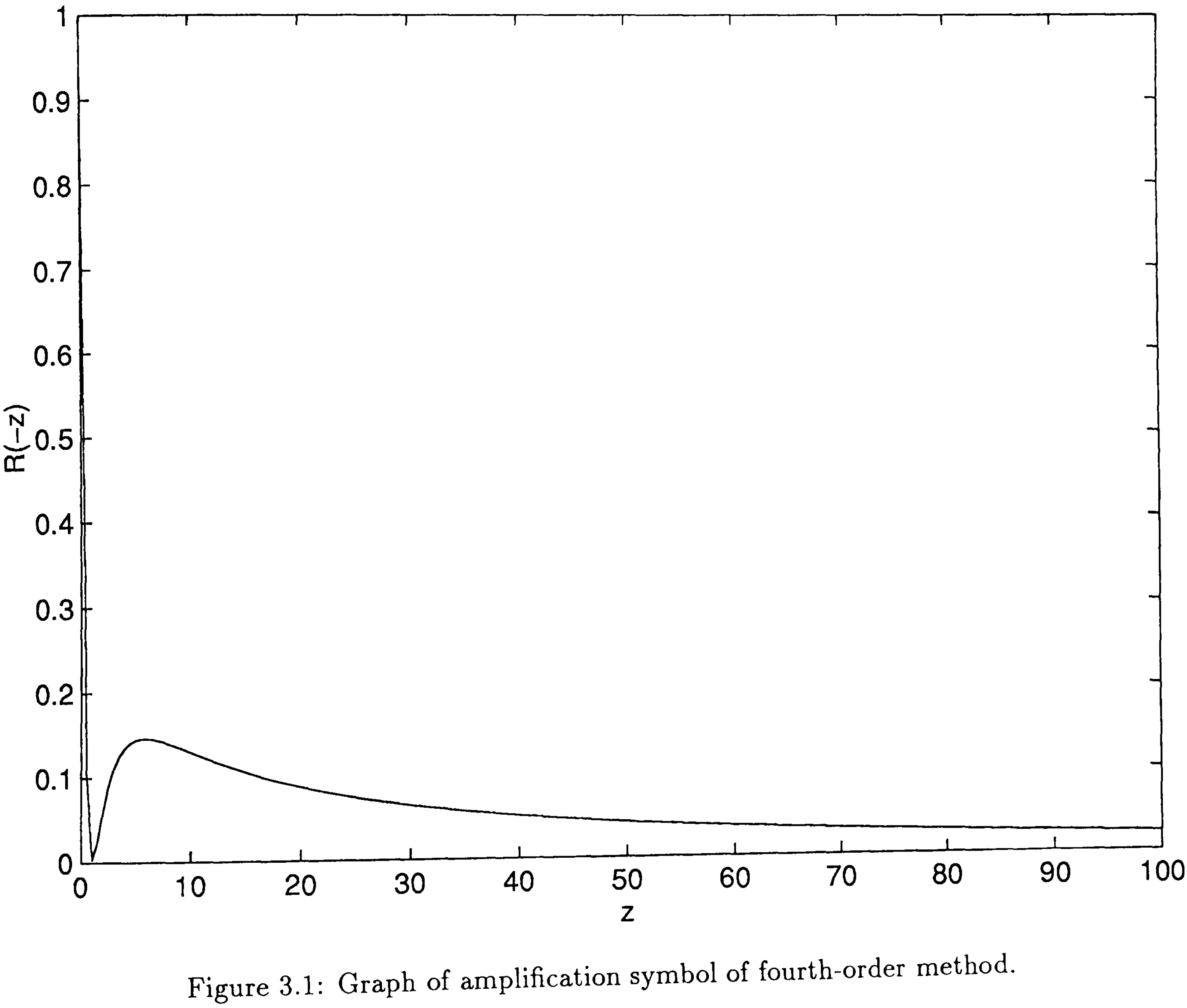

Figure 3.1: Graph of amplification symbol of fourth-order method.

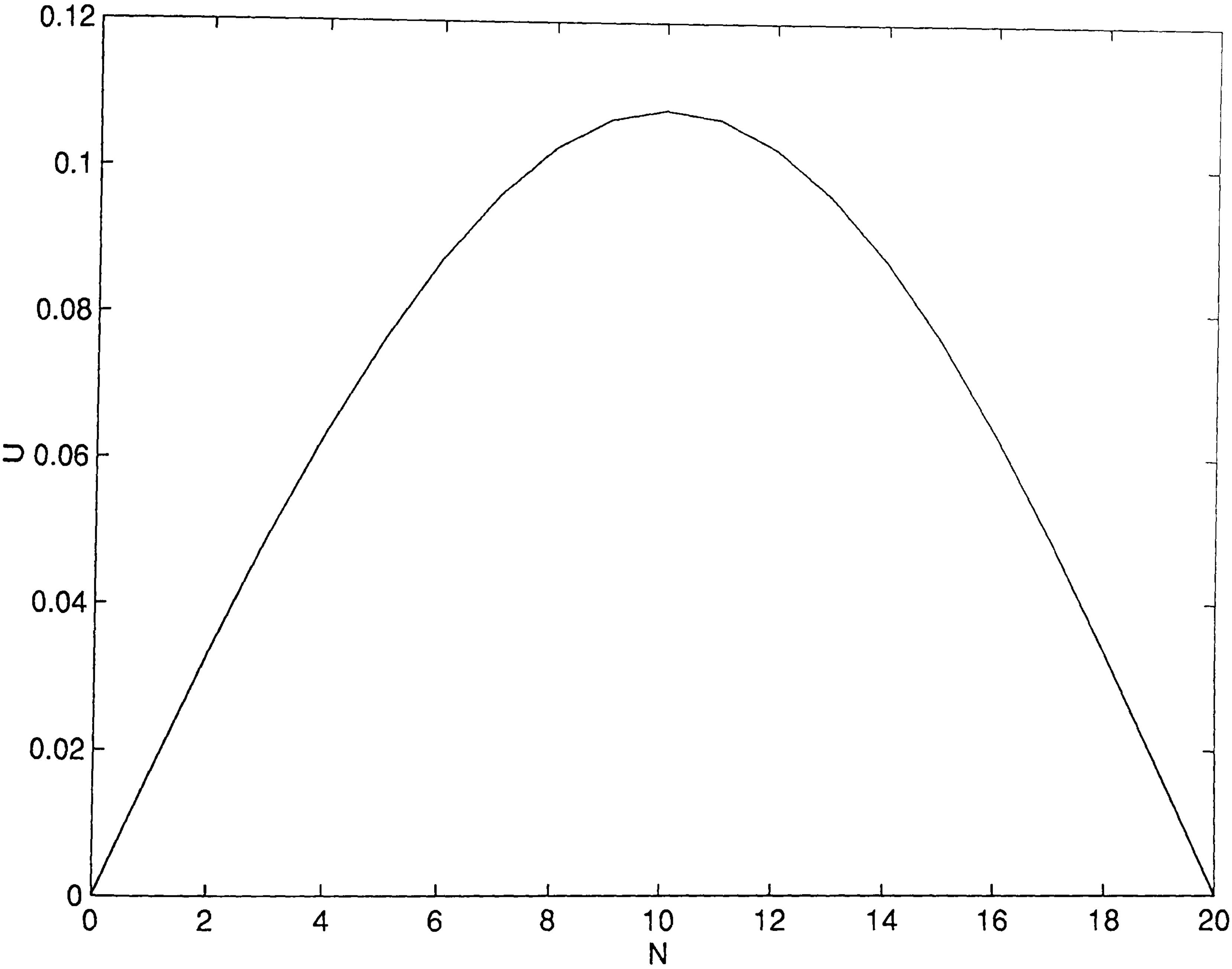

Figure 3.2: Numerical solution of one dimensional heat equation when h=0.1 and l=0.1 at time t=1.

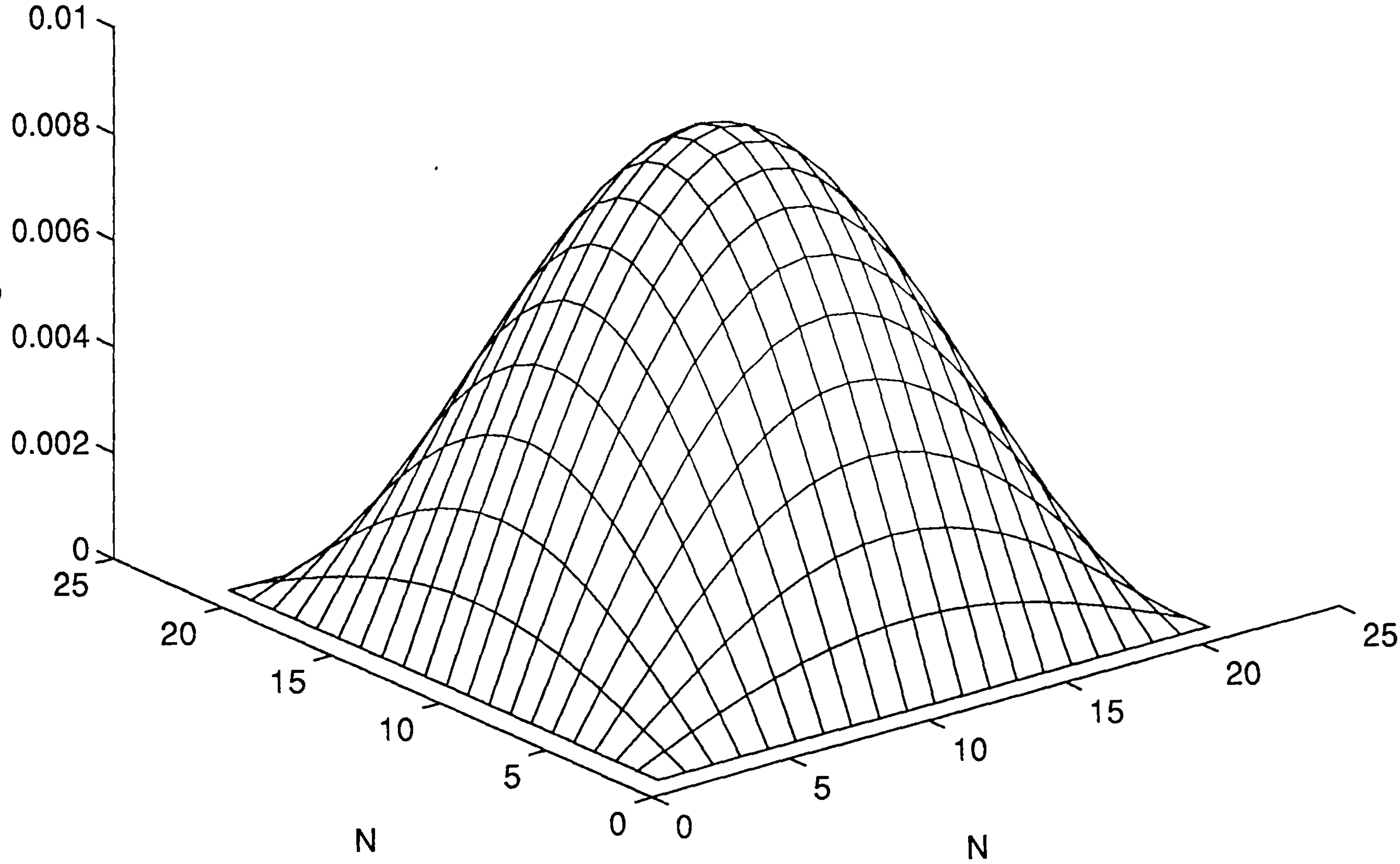

Figure 3.3: Numerical solution of two dimensional heat equation when h=0.1 and l=0.1 at t=1.

Chapter 4

Third-Order Numerical Methods for Time-Dependent Boundary-value Problems

4.1 Derivation of the methods

Suppose that (2.2) is non-homogeneous and

$$u(0,t) = f_1(t), \quad t > 0 \tag{4.1}$$

and

$$u(X,t) = f_2(t), \quad t > 0. \tag{4.2}$$

Then using the method developed in section 2.1 gives

$$\frac{d\mathbf{U}(t)}{dt} = A\,\mathbf{U}(t) + \mathbf{v}(t), \quad t > 0 \tag{4.3}$$

with initial distribution

$$\mathbf{U}(0) = \mathbf{g} \tag{4.4}$$

in which $\mathbf{U}(t) = [U_1(t), U_2(t), \ldots, U_N(t)]^T$, $\mathbf{g} = [g(h), g(2h), \ldots, g(Nh)]^T$ and $\mathbf{v}(t) = \frac{h^{-2}}{12}[11\,f_1(t), 0, 0, \ldots, 0, -f_2(t), -2\,f_2(t), 9\,f_2(t)]^T$, T denoting transpose, A is given by (2.21) and recurrence relation (2.23) takes the form

$$\mathbf{U}(t+l) = \exp(lA)\mathbf{U}(t) + \int_t^{t+l} \exp[(t+l-s)A]\mathbf{v}(s)ds, \quad t = 0, l, 2l, \ldots \quad (4.5)$$

To develop the method the matrix exponential function $exp(lA)$ will be approximated by (2.40) and following Twizell *et al.* (1996) the quadrature term will be approximated by

$$\int_t^{t+l} exp((t+l-s)A)\mathbf{v}(s)ds = W_1\mathbf{v}(s_1) + W_2\mathbf{v}(s_2) + W_3\mathbf{v}(s_3) \quad (4.6)$$

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

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

$$W_1 + W_2 + W_3 = M_1 \quad (4.7)$$

where

$$M_1 = A^{-1}(exp(lA) - I), \quad (4.8)$$

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

$$s_1W_1 + s_2W_2 + s_3W_3 = M_2 \quad (4.9)$$

where

$$M_2 = A^{-1}\left\{t\, exp(lA) - (t+l)\, I + A^{-1}(exp(lA) - I)\right\} \quad (4.10)$$

and

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

$$s_1^2W_1 + s_2^2W_2 + s_3^2W_3 = M_3 \quad (4.11)$$

where

$$\begin{aligned} M_3 &= A^{-1}\left\{t^2 exp(lA) - (t+l)^2 I + 2\,A^{-1}\{t\, exp(lA) - (t+l)\, I \right. \\ &+ \left. A^{-1}(exp(lA) - I)\}\right\}. \end{aligned} \quad (4.12)$$

Taking $s_1 = t$, $s_2 = t + \frac{l}{2}$, $s_3 = t + l$ and then solving (4.7), (4.9) and (4.11) simultaneously gives

$$W_1 = \frac{2}{l^2}\left\{(t^2 + \frac{3}{2}lt + \frac{l^2}{2})M_1 - (2t + \frac{3}{2}l)M_2 + M_3\right\}, \quad (4.13)$$

$$W_2 = \frac{-4}{l^2}\left\{(t^2 + lt)M_1 - (2t + l)M_2 + M_3\right\} \quad (4.14)$$

$$W_3 = \frac{2}{l^2}\left\{(t^2 + \frac{l}{2}t)M_1 - (2t + \frac{l}{2})M_2 + M_3\right\}. \quad (4.15)$$

Using (4.8), (4.10) and (4.12) in (4.13), (4.14) and (4.15) gives

$$\begin{aligned} W_1 &= \frac{2}{l^2}\Big[(t^2 + \frac{3}{2}lt + \frac{l^2}{2})A^{-1}(exp(lA) - I) \\ &- (2t + \frac{3}{2}l)A^{-1}\left\{t\,exp(lA) - (t+l)\,I + A^{-1}(exp(lA) - I)\right\} \\ &+ A^{-1}\Big\{t^2 exp(lA) - (t+l)^2 I + 2\,A^{-1}\{t\,exp(lA) - (t+l)\,I \\ &+ A^{-1}(exp(lA) - I)\}\Big\}\Big], \end{aligned} \quad (4.16)$$

$$\begin{aligned} W_2 &= \frac{-4}{l^2}\Big[(t^2 + lt)A^{-1}(exp(lA) - I) \\ &- (2t + l)A^{-1}\left\{t\,exp(lA) - (t+l)\,I + A^{-1}(exp(lA) - I)\right\} \\ &+ A^{-1}\Big\{t^2 exp(lA) - (t+l)^2 I + 2\,A^{-1}\{t\,exp(lA) - (t+l)\,I \\ &+ A^{-1}(exp(lA) - I)\}\Big\}\Big] \end{aligned} \quad (4.17)$$

and

$$\begin{aligned} W_3 &= \frac{2}{l^2}\Big[(t^2 + \frac{l}{2}t + \frac{l^2}{2})A^{-1}(exp(lA) - I) \\ &- (2t + \frac{l}{2})A^{-1}\left\{t\,exp(lA) - (t+l)\,I + A^{-1}(exp(lA) - I)\right\} \\ &+ A^{-1}\Big\{t^2 exp(lA) - (t+l)^2 I + 2\,A^{-1}\{t\,exp(lA) - (t+l)\,I \\ &+ A^{-1}(exp(lA) - I)\}\Big\}\Big] \end{aligned} \quad (4.18)$$

or

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

$$
\begin{aligned}
&- \quad (2t + \frac{3}{2}l)A^2 \left\{ t\, exp(lA) - (t+l)\, I + A^{-1}(exp(lA) - I) \right\} \\
&+ \quad A^2 \left\{ t^2 exp(lA) - (t+l)^2 I + 2\, A^{-1}\{t\, exp(lA) - (t+l)\, I \right. \\
&+ \quad \left. A^{-1}(exp(lA) - I)\}\right\} \Big], \qquad (4.\ 19)
\end{aligned}
$$

$$
\begin{aligned}
W_2 &= \frac{-4}{l^2}(A^{-1})^3 \Big[(t^2 + lt)A^2(exp(lA) - I) \\
&- \quad (2t + l)A^2 \left\{ t\, exp(lA) - (t+l)\, I + A^{-1}(exp(lA) - I) \right\} \\
&+ \quad A^2 \left\{ t^2 exp(lA) - (t+l)^2 I + 2\, A^{-1}\{t\, exp(lA) - (t+l)\, I \right. \\
&+ \quad \left. A^{-1}(exp(lA) - I)\}\right\} \Big] \qquad (4.\ 20)
\end{aligned}
$$

and

$$
\begin{aligned}
W_3 &= \frac{2}{l^2}(A^{-1})^3 \Big[(t^2 + \frac{l}{2}t + \frac{l^2}{2})A^2(exp(lA) - I) \\
&- \quad (2t + \frac{l}{2})A^2 \left\{ t\, exp(lA) - (t+l)\, I + A^{-1}(exp(lA) - I) \right\} \\
&+ \quad A^2 \left\{ t^2 exp(lA) - (t+l)^2 I + 2\, A^{-1}\{t\, exp(lA) - (t+l)\, I \right. \\
&+ \quad \left. A^{-1}(exp(lA) - I)\}\right\} \Big]. \qquad (4.\ 21)
\end{aligned}
$$

Then it is easy to show that

$$
\begin{aligned}
W_1 &= \frac{2}{l^2}(A^{-1})^3\{(\frac{l^2}{2}A^2 - \frac{3l}{2}A + 2I)\, exp(lA) - (\frac{l}{2}A + 2I)\} \qquad (4.\ 22) \\
W_2 &= -\frac{4}{l^2}(A^{-1})^3\, \{(2I - lA)\, exp(lA) - (2I + lA)\}, \qquad (4.\ 23) \\
W_3 &= \frac{2}{l^2}(A^{-1})^3\{(2I - \frac{l}{2}A)exp(lA) - (2I + \frac{3l}{2}A + \frac{l^2}{2}A^2)\}. \qquad (4.\ 24)
\end{aligned}
$$

Using (2.28)

$$
exp(lA) = G^{-1}N \qquad (4.\ 25)
$$

where

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

and

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

in (4.22)-(4.24) gives

$$W_1 = \frac{l}{6}\{(I + (4 - 9a_1 + 12a_2)lA\} G^{-1}, \quad (4.26)$$

$$W_2 = \frac{2l}{3}\{(I - (1 - 3a_1 + 6a_2)lA\} G^{-1}, \quad (4.27)$$

and

$$W_3 = \frac{l}{6}\{(I + (3 - 9a_1 + 12a_2)lA + (1 - 3a_1 + 6a_2)l^2A^2\} G^{-1}. \quad (4.28)$$

Hence (4.5) can be written as

$$\mathbf{U}(t+l) = exp(lA)\mathbf{U}(t) + W_1\mathbf{v}(t) + W_2\mathbf{v}(t + \frac{l}{2}) + W_3\mathbf{v}(t+l). \quad (4.29)$$

4.2 Algorithm

Let r_1, r_2 and r_3 be the real zeros of the denominator of $E_3(\theta)$; then

$$G = (I - \frac{l}{r_1}A)(I - \frac{l}{r_2}A)(I - \frac{l}{r_3}A) \quad (4.30)$$

and

$$exp(lA)\mathbf{U}(t) = \left\{p_1(I - \frac{l}{r_1}A)^{-1} + p_2(I - \frac{l}{r_2}A)^{-1} + p_3(I - \frac{l}{r_3}A)^{-1}\right\}\mathbf{U}(t) \quad (4.31)$$

where

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

$$W_1\mathbf{v}(t) = \frac{l}{6}\left\{p_4(I - \frac{l}{r_1}A)^{-1} + p_5(I - \frac{l}{r_2}A)^{-1} + p_6(I - \frac{l}{r_3}A)^{-1}\right\}\mathbf{v}(t), \quad (4.32)$$

where

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

$$W_2\mathbf{v}(t+\frac{l}{2}) = \frac{2l}{3}\left\{p_7(I-\frac{l}{r_1}A)^{-1} + p_8(I-\frac{l}{r_2}A)^{-1} + p_9(I-\frac{l}{r_3}A)^{-1}\right\}\mathbf{v}(t+\frac{l}{2}), \tag{4.33}$$

where

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

and

$$W_3\mathbf{v}(t+l) = \frac{l}{6}\left\{p_{10}(I-\frac{l}{r_1}A)^{-1} + p_{11}(I-\frac{l}{r_2}A)^{-1} + p_{12}(I-\frac{l}{r_3}A)^{-1}\right\}\mathbf{v}(t+l) \tag{4.34}$$

where

$$p_{9+j} = \frac{1+(3-9a+12b)r_j+(1-3a+6b)r_j^2}{\prod_{\substack{i=1\\ i\neq j}}^{3}(1-\frac{r_j}{r_i})}, \quad j=1,2,3.$$

So

$$\begin{aligned}\mathbf{U}(t+l) &= A_1^{-1}\{p_1\mathbf{U}(t)+\frac{l}{6}(p_4\mathbf{v}(t)+4p_7\mathbf{v}(t+\frac{l}{2})+p_{10}\mathbf{v}(t+l))\}\\ &+ A_2^{-1}\{p_2\mathbf{U}(t)+\frac{l}{6}(p_5\mathbf{v}(t)+4p_8\mathbf{v}(t+\frac{l}{2})+p_{11}\mathbf{v}(t+l))\}\\ &+ A_3^{-1}\{p_3\mathbf{U}(t)+\frac{l}{6}(p_6\mathbf{v}(t)+4p_9\mathbf{v}(t+\frac{l}{2})+p_{12}\mathbf{v}(t+l))\},\end{aligned} \tag{4.35}$$

where

$$A_i = I - \frac{l}{r_i}A, \quad i=1,2,3. \tag{4.36}$$

Hence

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

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

$$A_1\mathbf{y}_1 = p_1\mathbf{U}(t)+\frac{l}{6}\{p_4\mathbf{v}(t)+4p_7\mathbf{v}(t+\frac{l}{2})+p_{10}\mathbf{v}(t+l)\}. \tag{4.38}$$

$$A_2\mathbf{y}_2 = p_2\mathbf{U}(t) + \frac{l}{6}\{p_5\mathbf{v}(t) + 4p_8\mathbf{v}(t+\frac{l}{2}) + p_{11}\mathbf{v}(t+l)\} \qquad (4.39)$$

and

$$A_3\mathbf{y}_3 = p_3\mathbf{U}(t) + \frac{l}{6}\{p_6\mathbf{v}(t) + 4p_9\mathbf{v}(t+\frac{l}{2}) + p_{12}\mathbf{v}(t+l)\} \qquad (4.40)$$

respectively. Some details of this algorithm are given in Table 4.1.

4.3 Numerical Examples

4.3.1 Example 1

Consider the one space variable partial differential equation (2.1)

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial t^2}, \quad 0 < x < 1, \quad t > 0. \qquad (4.41)$$

subject to the boundary conditions

$$u(0,t) = 0, \quad t > 0, \qquad (4.42)$$

$$u(1,t) = e^{-\frac{\pi^2}{4}t}, \quad t > 0, \qquad (4.43)$$

and the initial condition

$$u(x,0) = sin(\frac{\pi}{2}x), \quad 0 \le x \le 1. \qquad (4.44)$$

This problem, which has theoretical solution

$$u(x,t) = e^{-\frac{\pi^2}{4}t} sin(\frac{\pi}{2}x) \qquad (4.45)$$

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 shown in Figure 4.1. Using the algorithm developed in section 4.2 with the informations given in section 2.8 of Chapter 2 the problem {(4.41)–(4.44)} is solved for

$$h = 0.125, 0.1, 0.05, 0.025, 0.0125, 0.01, 0.005, 0.001$$

using

$$l = 0.125, 0.01, 0.05, 0.025, 0.0125, 0.01, 0.005, 0.001.$$

The numerical solution for $h = 0.1$ and $l = 0.005$ at the time $t = 1.$ is depicted in Figure 4.2. 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 $t = 1.0$, are given with positions in Table 4.2.

4.3.2 Example 2

Consider again the one space variable partial differential equation (2.1)

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial t^2}, \quad 0 < x < 1, \quad t > 0. \qquad (4.46)$$

subject to the boundary conditions

$$u(0,t) = t, \quad t > 0, \qquad (4.47)$$

$$u(1,t) = 0, \quad t > 0, \qquad (4.48)$$

and the initial condition

$$u(x,0) = 1, \quad 0 \leq x \leq 1. \qquad (4.49)$$

This problem, which has theoretical solution

$$\begin{aligned} u(x,t) &= (1-x)t - \frac{1}{6}(x^3 - 3x^2 + 2x) \\ &+ \sum_{n=1}^{\infty} 2\left\{1 - (-1)^n + \frac{1}{n^2\pi^2}\right\} e^{(-n^2\pi^2 t)} \frac{sin(n\pi x)}{n\pi} \end{aligned} \qquad (4.50)$$

(Lawson and Swayne, (1976)) has discontinuities between the initial conditions and the boundary conditions at $x = 0$ and $x = 1$. The theoretical solution at time $t = 1.0$ is shown in Figure 4.3.

Using once again the algorithm developed in Section 4.2, together with the informations given in section 2.8 of Chapter 2, the problem $\{(4.46)$–$(4.49)\}$ is solved for

$$h = 0.125, 0.1, 0.05, 0.025, 0.0125, 0.01, 0.005, 0.001$$

using

$$l = 0.125, 0.01, 0.05, 0.025, 0.0125, 0.01, 0.005, 0.001.$$

The numerical solution for $h = 0.1$ and $l = 0.005$ at the time $t = 1.$ is depicted in Figure 4.4. In these experiments, when bigger values of h and l are used the method behaves smoothly over the whole interval $0 \leq x \leq 1$ but oscillations are observed for smaller values. The accuracy is also affected by smaller values of h and l because the error grows rapidly near the end where growing time-dependent boundary condition is given. Maximum errors, with positions, at time $t = 1.0$ are giveg in Table 4.4.

Table 4.1: Algorithm 1

Steps	Processor 1	Processor 2	Processor 3
1 Input	$l, r_1, \mathbf{U}_0, A$ p_1, p_4, p_7, p_{10}	$l, r_2, \mathbf{U}_0, A$ p_2, p_5, p_8, p_{11}	$l, r_3, \mathbf{U}_0, A$ p_3, p_6, p_9, p_{12}
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	$\mathbf{v}(t)$, $\mathbf{v}(t + \frac{l}{2})$ $\mathbf{v}(t + l)$	$\mathbf{v}(t)$, $\mathbf{v}(t + \frac{l}{2})$ $\mathbf{v}(t + l)$	$\mathbf{v}(t)$, $\mathbf{v}(t + \frac{l}{2})$ $\mathbf{v}(t + l)$
5 Using	$\mathbf{w}_1(t) = \frac{l}{6}(p_4\mathbf{v}(t) + 4p_7\mathbf{v}(t + \frac{l}{2}) + p_{10}\mathbf{v}(t + l))$	$\mathbf{w}_2(t) = \frac{l}{6}(p_5\mathbf{v}(t) + 4p_8\mathbf{v}(t + \frac{l}{2}) + p_{11}\mathbf{v}(t + l))$	$\mathbf{w}_3(t) = \frac{l}{6}(p_6\mathbf{v}(t) + 4p_9\mathbf{v}(t + \frac{l}{2}) + p_{12}\mathbf{v}(t + l))$
6 Solve	$L_1U_1\mathbf{y}_1(t) = p_1\mathbf{U}(t) + \mathbf{w}_1(t)$	$L_2U_2\mathbf{y}_2(t) = p_2\mathbf{U}(t) + \mathbf{w}_2(t)$	$L_3U_3\mathbf{y}_3(t) = p_3\mathbf{U}(t) + \mathbf{w}_3(t)$
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 $t = 1.0$

N	7	9	19	39
h	0.125	0.1	0.05	0.025
l=0.125	0.58272D-4 5	0.51949D-4 6	0.46097D-4 12	0.45367D-4 24
l=0.1	0.38016D-4 4	0.31546D-4 6	0.25715D-4 12	0.25009D-4 25
l=0.05	0.17834D-4 4	0.10664D-4 5	0.45220D-5 12	0.38144D-5 25
l=0.025	0.14849D-4 4	0.67815D-5 5	0.13833D-5 10	0.62244D-6 25
l=0.0125	0.14441D-4 4	0.72748D-5 5	0.98359D-6 9	0.18544D-6 21
l=0.01	0.14414D-4 4	0.72469D-5 5	0.95764D-6 9	0.15737D-6 20
l=0.005	0.14395D-4 4	0.72287D-5 5	0.94103D-6 9	0.13982D-6 19
l=0.001	0.14468D-4 4	0.73010D-5 5	0.10112D-5 9	0.21163D-6 20

continued

Table 4.3: Continuation of Table 4.2

N	79	99	199	999
h	0.0125	0.01	0.005	0.001
l=0.125	0.45299D-4 49	0.45292D-4 61	0.45286D-4 122	0.45286D-4 614-614
l=0.1	0.24923D-4 49	0.24918D-4 62	0.24913D-4 123-124	0.24914D-4 616-618
l=0.05	0.37282D-5 51	0.37221D-5 64	0.37165D-5 128	0.37170D-5 639-641
l=0.025	0.53597D-6 53	0.53010D-6 66	0.52479D-6 133	0.52520D-6 665-667
l=0.0125	0.89028D-7 51	0.82983D-7 66	0.77651D-7 135	0.78020D-7 675-677
l=0.01	0.58022D-7 48	0.51627D-7 63	0.45989D-7 132	0.44489D-7 665-666
l=0.005	0.38097D-7 42	0.31095D-7 54	0.24733D-7 113	0.22840D-7 569-571
l=0.001	0.11104D-6 43	0.10410D-6 54	0.97680D-7 109	0.96164D-7 548-549

Positions are shown by the space steps

Table 4.4: Maximum errors for Example 2 at the time t=1.0

N	7	9	19	39
h	0.125	0.1	0.05	0.025
l=0.125	0.18614D-4 4	0.18712D-4 5	0.18863D-4 10	0.18876D-4 20
l=0.1	0.10491D-4 4	0.10598D-4 5	0.10762D-4 10	0.10776D-4 20
l=0.05	0.13915D-5 4	0.15079D-5 5	0.16853D-5 10	0.17013D-5 20
l=0.025	-0.13522D-6 5	0.25672D-6 1	-0.34734D-6 1	-0.34694D-6 2
l=0.0125	-0.30550D-6 5	0.20389D-6 1	-0.37375D-6 1	-0.37376D-6 2
l=0.01	-0.31094D-6 5	0.20407D-6 1	-0.37349D-6 1	-0.37310D-6 2
l=0.005	-0.28193D-6 5	0.22383D-6 1	-0.36259D-6 1	-0.36220D-6 2
l=0.001	0.30400D-6 3	0.43278D-6 3	0.54700D-6 8	0.55961D-6 16

continued

Table 4.5: Continuation of Table 4.4

N	79	99	199	999
h	0.0125	0.01	0.005	0.001
l=0.125	0.18877D-4 40	0.18877D-4 50	0.18877D-4 100	0.18893D-4 498
l=0.1	0.10777D-4 40	0.10778D-4 50	0.10778D-4 100	0.10798D-4 497-498
l=0.05	0.17023D-5 40	0.17025D-5 50	0.16314D-5 1	0.24599D-5 3
l=0.025	-0.12074D-5 1	-0.11707D-5 1	0.16093D-5 1	0.24467D-5 3
l=0.0125	-0.12139D-5 1	-0.11760D-5 1	0.16068D-5 1	0.24452D-5 3
l=0.01	-0.12138D-5 1	-0.11759D-5 1	0.16068D-5 1	0.24450D-5 3
l=0.005	-0.12109D-5 1	-0.11736D-5 1	0.16080D-5 1	0.24457D-5 3
l=0.001	-0.11830D-5 1	-0.11512D-5 1	0.16192D-5 1	0.24525D-5 3

Positions are shown by the space steps

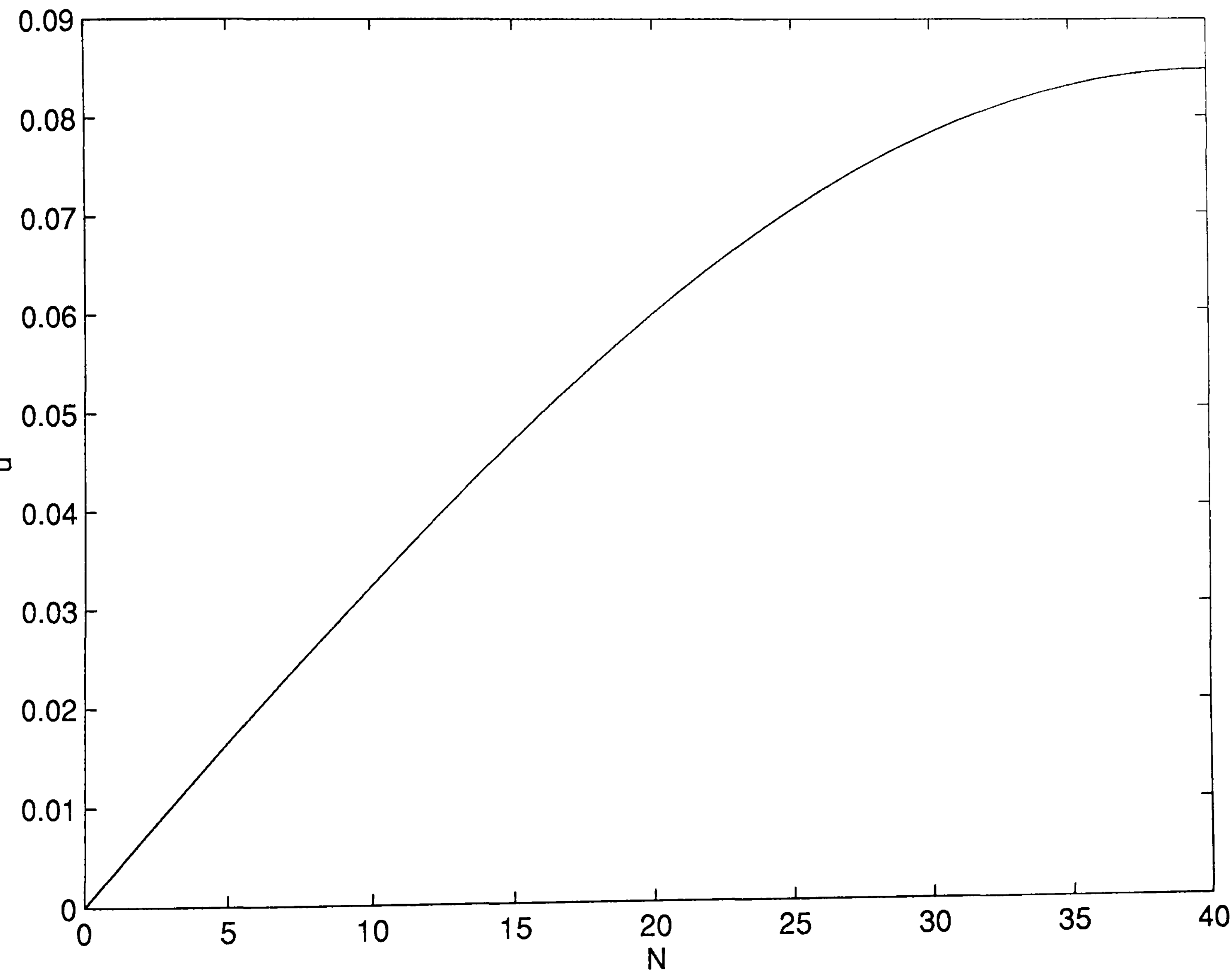

Figure 4.1: Theoretical solution of numerical example 1 at time t=1.

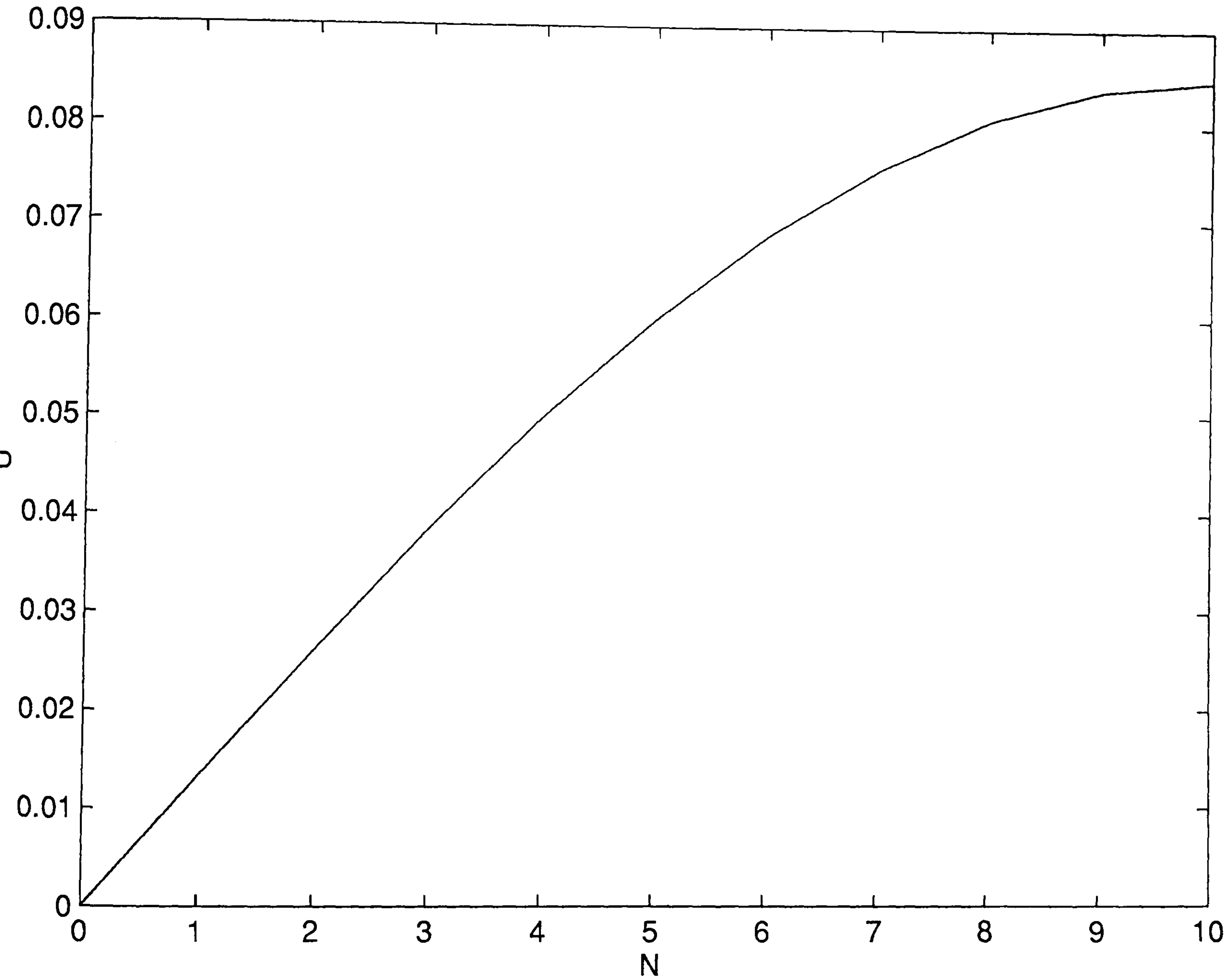

Figure 4.2: Numerical solution of numerical example 1 when h=0.1 and l=0.005 at time t=1.

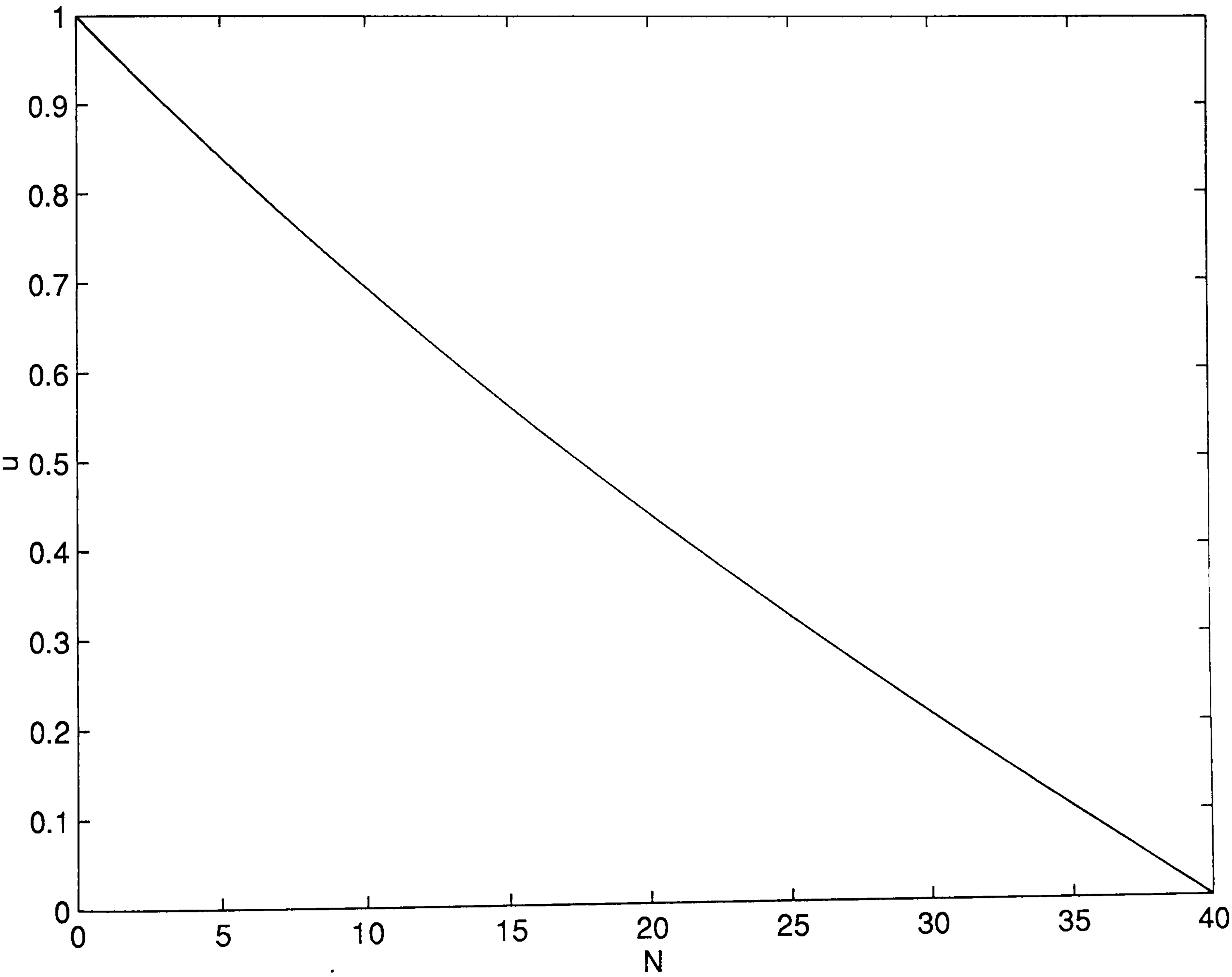

Figure 4.3: Theoretical solution of numerical example 2 at time t=1.

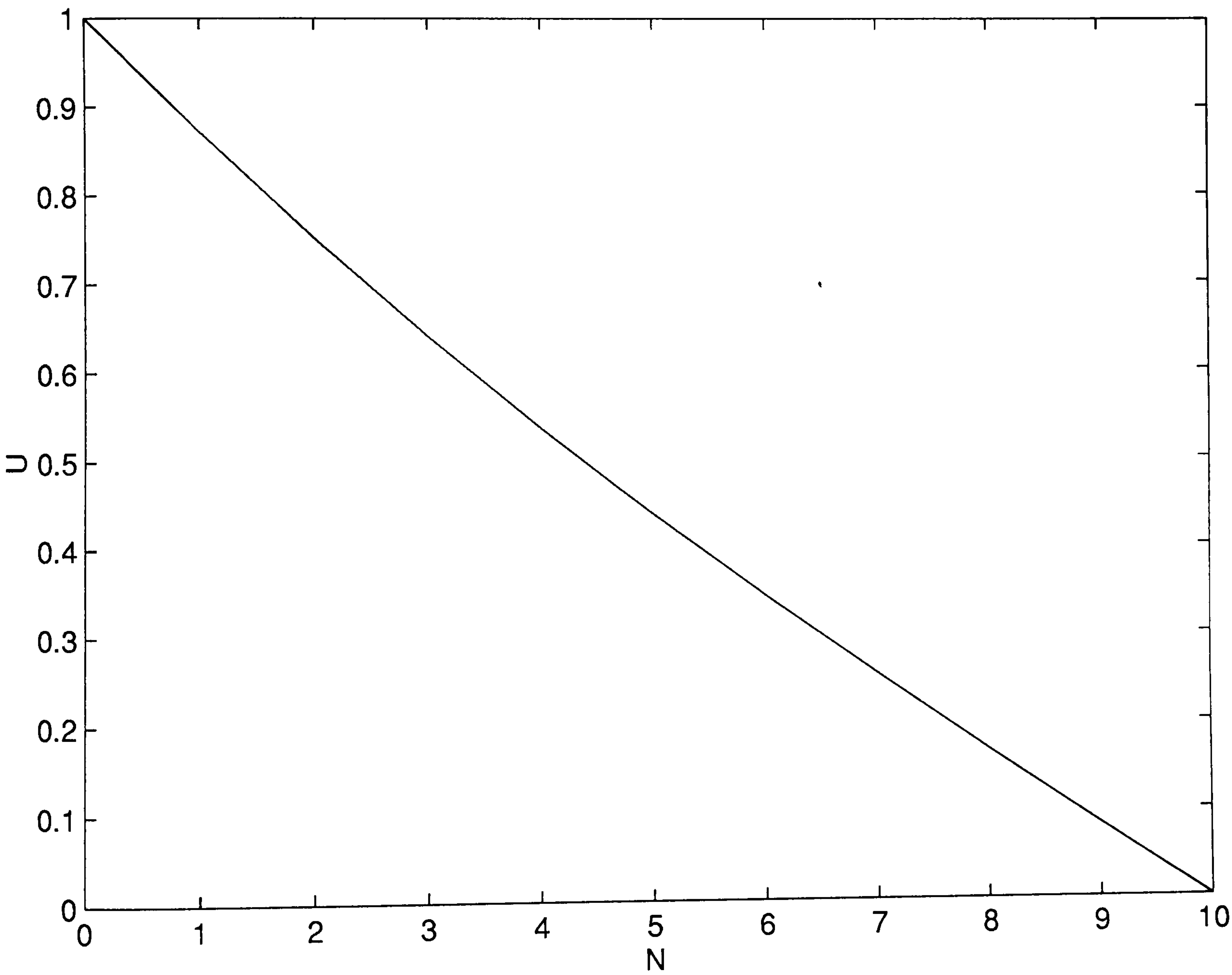

Figure 4.4: Numerical solution of numerical example 2 when h=0.1 and l=0.005 at time t=1.

Chapter 5

Fourth-order Numerical Methods for Time-Dependent Boundary-value Problems

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5.1 Derivation of the methods

In this chapter $exp(lA)$ is denoted by E for convenience. Consider the problem {(3.1)–(3.4)} with

$$u(0,t) = f_1(t), \quad t > 0 \tag{5.1}$$

and

$$u(X,t) = f_2(t), \quad t > 0 \tag{5.2}$$

Then using the method developed in section 3.1 gives

$$\frac{d\mathbf{U}(t)}{dt} = A\,\mathbf{U}(t) + \mathbf{v}(t), \quad t > 0 \tag{5.3}$$

with initial distribution

$$\mathbf{U}(0) = \mathbf{g} \tag{5.4}$$

in which

$$\mathbf{U}(t) = [U_1(t), U_2(t), \ldots, U_N(t)]^T,$$

$$\mathbf{g} = [g(h), g(2h), \ldots, g(Nh)]^T$$

and

$$\mathbf{v}(t) = \frac{h^{-2}}{12}[9\,f_1(t), -f_1(t), 0, 0, \ldots, 0, -f_2(t), 9\,f_2(t)]^T,$$

T denoting transpose, A is given by (3.20) and recurrence relation (3.22) takes the form

$$\mathbf{U}(t+l) = \exp(lA)\mathbf{U}(t) + \int_t^{t+l} \exp[(t+l-s)A]\mathbf{v}(s)ds, \;\; t = 0, l, 2l, \ldots \quad (5.5)$$

To develop the method the matrix exponential function $exp(lA)$ will be approximated by (3.34) and the quadrature term will be approximated (as in Chapter 4) by

$$\int_t^{t+l} exp((t+l-s)A)\mathbf{v}(s)ds = W_1\mathbf{v}(s_1) + W_2\mathbf{v}(s_2) + W_3\mathbf{v}(s_3) + W_4\mathbf{v}(s_4) \quad (5.6)$$

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

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

$$W_1 + W_2 + W_3 + W_4 = M_1, \quad (5.7)$$

where

$$M_1 = A^{-1}(E - I), \quad (5.8)$$

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

$$s_1W_1 + s_2W_2 + s_3W_3 + s_4W_4 = M_2, \quad (5.9)$$

where

$$M_2 = A^{-1}\{t\,E - (t+l)\,I + A^{-1}(E - I)\} \quad (5.10)$$

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

$$s_1^2W_1 + s_2^2W_2 + s_3^2W_3 + s_4^2W_4 = M_3, \quad (5.11)$$

where

$$M_3 = A^{-1}\Big\{t^2E-(t+l)^2I+2\,A^{-1}\{t\,E-(t+l)\,I + A^{-1}(E-I)\}\Big\} \qquad (5.12)$$

and

(iv) <u>when $\mathbf{v}(s) = [s^3, s^3, \ldots, s^3]^T$</u>

$$s_1^3W_1+s_2^3W_2+s_3^3W_3+s_4^3W_4 = M_4, \qquad (5.13)$$

where

$$M_4 = A^{-1}\Big\{t^3E-(t+l)^3I+3\,A^{-1}\{t^2\,E-(t+l)^2\,I + 2\,A^{-1}\{t\,E-(t+l)\,I+A^{-1}(E-I)\}\}\Big\}. \qquad (5.14)$$

Taking $s_1 = t$, $s_2 = t+\frac{l}{3}$, $s_3 = t+\frac{2}{3}l$, $s_4 = t+l$ and then solving (5.7), (5.9), (5.11) and (5.13) simultaneously gives

$$\begin{aligned} W_1 &= \frac{9}{2l^3}\Big[(t^3+2lt^2+\frac{11}{9}l^2t+\frac{2}{9}l^3)M_1 \\ &- (3t^2+4lt+\frac{11}{9}l^2)M_2 \\ &+ (3t+2l)M_3-M_4\Big], \end{aligned} \qquad (5.15)$$

$$\begin{aligned} W_2 &= -\frac{27}{2l^3}\Big\{(t^3+\frac{5}{3}lt^2+\frac{2}{3}l^2t)M_1 \\ &- (3t^2+\frac{10}{3}lt+\frac{2}{3}l^2)M_2 \\ &+ (3t+\frac{5}{3}l)M_3-M_4\Big\}, \end{aligned} \qquad (5.16)$$

$$\begin{aligned} W_3 &= \frac{27}{2l^3}\Big\{(t^3+\frac{4}{3}lt^2+\frac{1}{3}l^2t)M_1 \\ &- (3t^2+\frac{8}{3}lt+\frac{1}{3}l^2)M_2 \\ &+ (3t+\frac{4}{3}l)M_3-M_4\Big\} \end{aligned} \qquad (5.17)$$

and

$$
\begin{aligned}
W_4 &= -\frac{9}{2l^3}\Big[(t^3 + lt^2 + \frac{2}{9}l^2 t)M_1 \\
&- (3t^2 + 2lt + \frac{2}{9}l^2)M_2 \\
&+ (3t + l)M_3 - M_4\Big]. \qquad (5.18)
\end{aligned}
$$

Using (5.8), (5,10), (5.12) and (5.14) in (5.15)–(5.18) gives

$$
\begin{aligned}
W_1 &= \frac{9}{2l^3}\Big[(t^3 + 2lt^2 + \frac{11}{9}l^2 t + \frac{2}{9}l^3)A^{-1}(E - I) \\
&- (3t^2 + 4lt + \frac{11}{9}l^2)A^{-1}\{t\,E - (t+l)\,I + A^{-1}(E - I)\} \\
&+ (3t + 2l)A^{-1}\Big\{t^2 E - (t+l)^2 I + 2\,A^{-1}\{t\,E - (t+l)\,I \\
&+ A^{-1}(E - I)\}\Big\} \\
&- A^{-1}\Big\{t^3 E - (t+l)^3 I + 3\,A^{-1}\{t^2\,E - (t+l)^2\,I \\
&+ 2\,A^{-1}\{t\,E - (t+l)\,I + A^{-1}(E - I)\}\}\Big\}\Big], \qquad (5.19)
\end{aligned}
$$

$$
\begin{aligned}
W_2 &= -\frac{27}{2l^3}\Big[(t^3 + \frac{5}{3}lt^2 + \frac{2}{3}l^2 t)A^{-1}(E - I) \\
&- (3t^2 + \frac{10}{3}lt + \frac{2}{3}l^2)A^{-1}\{t\,E - (t+l)\,I + A^{-1}(E - I)\} \\
&+ (3t + \frac{5}{3}l)A^{-1}\Big\{t^2 E - (t+l)^2 I + 2\,A^{-1}\{t\,E - (t+l)\,I \\
&+ A^{-1}(E - I)\}\Big\} \\
&- A^{-1}\Big\{t^3 E - (t+l)^3 I + 3\,A^{-1}\{t^2\,E - (t+l)^2\,I \\
&+ 2\,A^{-1}\{t\,E - (t+l)\,I + A^{-1}(E - I)\}\}\Big\}\Big], \qquad (5.20)
\end{aligned}
$$

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

$$
\begin{aligned}
&- \quad A^{-1}\Big\{t^3E-(t+l)^3I+3\,A^{-1}\{t^2\,E-(t+l)^2\,I\\
&+ \quad 2\,A^{-1}\{t\,E-(t+l)\,I+A^{-1}(E-I)\}\}\Big\}\Big]
\end{aligned} \qquad (5.21)
$$

and

$$
\begin{aligned}
W_4 &= -\frac{9}{2l^3}\Big[(t^3+lt^2+\frac{2}{9}l^2t)A^{-1}(E-I)\\
&- (3t^2+2lt+\frac{2}{9}l^2)A^{-1}\{t\,E-(t+l)\,I+A^{-1}(E-I)\}\\
&+ (3t+l)A^{-1}\Big\{t^2E-(t+l)^2I+2\,A^{-1}\{t\,E-(t+l)\,I\\
&+ A^{-1}(E-I)\}\Big\}\\
&- A^{-1}\Big\{t^3E-(t+l)^3I+3\,A^{-1}\{t^2\,E-(t+l)^2\,I\\
&+ 2\,A^{-1}\{t\,E-(t+l)\,I+A^{-1}(E-I)\}\}\Big\}\Big].
\end{aligned} \qquad (5.22)
$$

Simplifying these relations gives

$$
\begin{aligned}
W_1 &= \frac{9}{2l^3}(A^{-1})^4\Big\{6I+2lA+\frac{2}{9}l^2A^2\\
&- (6I-4lA+\frac{11}{9}l^2A^2-\frac{2}{9}l^3A^3)E\Big\}, \qquad (5.23)\\
W_2 &= -\frac{27}{2l^3}(A^{-1})^4\Big\{6I+\frac{8}{3}lA+\frac{1}{3}l^2A^2\\
&- (6I-\frac{10}{3}lA+\frac{2}{3}l^2A^2)E\Big\}, \qquad (5.24)\\
W_3 &= \frac{27}{2l^3}(A^{-1})^4\Big\{6I+\frac{10}{3}lA+\frac{2}{3}l^2A^2\\
&- (6I-\frac{8}{3}lA+\frac{1}{3}l^2A^2)E\Big\}, \qquad (5.25)\\
W_4 &= -\frac{9}{2l^3}(A^{-1})^4\Big\{6I+4lA+\frac{11}{9}l^2A^2+\frac{2}{9}l^3A^3\\
&- (6I-2lA+\frac{2}{9}l^2A^2)E\Big\}, \qquad (5.26)
\end{aligned}
$$

Using

$$E = exp(lA) = P\,Q$$

where

$$P = \left(I - a_1lA + a_2l^2A^2 - a_3l^3A^3 + (-\frac{1}{24}+\frac{a_1}{6}-\frac{a_2}{2}+a_3)l^4A^4\right)^{-1}$$

and

$$Q = \left(I + (1-a_1)lA + (\frac{1}{2} - a_1 + a_2)l^2A^2 + (\frac{1}{6} - \frac{a_1}{2} + a_2 - a_3)l^3A^3\right)$$

in (5.23)–(5.26) it is easy to obtain

$$\begin{aligned} W_1 &= \frac{l}{24}\{3I - (19 - 78a_1 + 216a_2 - 324a_3)lA \\ &+ (3 - 8a_1 + 12a_2)l^2A^2\}\, P, \end{aligned} \qquad (5.27)$$

$$\begin{aligned} W_2 &= \frac{3l}{16}\{2I + (16 - 56a_1 + 144a_2 - 216a_3)lA \\ &+ (1 - 4a_1 + 12a_2 - 24a_3)l^2A^2\}\, P, \end{aligned} \qquad (5.28)$$

$$\begin{aligned} W_3 &= \frac{3l}{8}\{I - (7 - 26a_1 + 72a_2 - 108a_3)lA \\ &- (1 - 4a_1 + 12a_2 - 24a_3)l^2A^2\}\, P, \end{aligned} \qquad (5.29)$$

$$\begin{aligned} W_4 &= \frac{l}{48}\{6I + (44 - 168a_1 + 432a_2 - 648a_3)lA \\ &+ (11 - 44a_1 + 132a_2 - 216a_3)l^2A^2 \\ &+ (2 - 8a_1 + 24a_2 - 48a_3)l^3A^3\}\, P. \end{aligned} \qquad (5.30)$$

Hence (5.5) becomes

$$\mathbf{U}(t+l) = E\mathbf{U}(t) + W_1\mathbf{v}(t) + W_2\mathbf{v}(t+\frac{l}{3}) + W_3\mathbf{v}(t+\frac{2l}{3}) + W_4\mathbf{v}(t+l) \qquad (5.31)$$

5.2 Algorithm

Let r_1, r_2, r_3 and r_4 be the real zeros of the denominator of $E_4(\theta)$ then

$$P^{-1} = (I - \frac{l}{r_1}A)(I - \frac{l}{r_2}A)(I - \frac{l}{r_3}A)(I - \frac{l}{r_4}A) \qquad (5.32)$$

and

$$\begin{aligned} E\mathbf{U}(t) &= \left\{p_1(I - \frac{l}{r_1}A)^{-1} + p_2(I - \frac{l}{r_2}A)^{-1} + p_3(I - \frac{l}{r_3}A)^{-1}\right. \\ &+ \left. p_4(I - \frac{l}{r_4}A)^{-1}\right\}\mathbf{U}(t), \end{aligned} \qquad (5.33)$$

where

$$p_j = \frac{1 + (1-a)r_j + (\frac{1}{2} - a + b)r_j^2 + (\frac{1}{6} - \frac{a}{2} + b - c)r_j^3}{\prod^4_{\substack{i=1\\ i \neq j}} (1 - \frac{r_j}{r_i})},$$

j=1,2,3,4

$$\begin{aligned} W_1 \mathbf{v}(t) &= \frac{l}{24}\left\{ p_5(I - \frac{l}{r_1}A)^{-1} + p_6(I - \frac{l}{r_2}A)^{-1} + p_7(I - \frac{l}{r_3}A)^{-1} \right. \\ &+ \left. p_8(I - \frac{l}{r_4}A)^{-1} \right\} \mathbf{v}(t), \qquad (5.34) \end{aligned}$$

where

$$p_{4+j} = \frac{3 + (-19 + 78a - 216b + 324c)r_j + (3 - 8a + 12b)r_j^2}{\prod^4_{\substack{i=1\\ i \neq j}} (1 - \frac{r_j}{r_i})},$$

j=1,2,3,4

$$\begin{aligned} W_2 \mathbf{v}(t + \frac{l}{3}) &= \frac{3l}{16}\left\{ p_9(I - \frac{l}{r_1}A)^{-1} + p_{10}(I - \frac{l}{r_2}A)^{-1} + p_{11}(I - \frac{l}{r_3}A)^{-1} \right. \\ &+ \left. p_{12}(I - \frac{l}{r_4}A)^{-1} \right\} \mathbf{v}(t + \frac{l}{3}), \qquad (5.35) \end{aligned}$$

where

$$p_{8+j} = \frac{2 + (16 - 56a + 144b - 216c)r_j + (1 - 4a + 12b - 24c)r_j^2}{\prod^4_{\substack{i=1\\ i \neq j}} (1 - \frac{r_j}{r_i})},$$

j=1,2,3,4

$$\begin{aligned} W_3 \mathbf{v}(t + \frac{2l}{3}) &= \frac{3l}{8}\left\{ p_{13}(I - \frac{l}{r_1}A)^{-1} + p_{14}(I - \frac{l}{r_2}A)^{-1} + p_{15}(I - \frac{l}{r_3}A)^{-1} \right. \\ &+ \left. p_{16}(I - \frac{l}{r_4}A)^{-1} \right\} \mathbf{v}(t + \frac{2l}{3}) \qquad (5.36) \end{aligned}$$

where

$$p_{12+j} = \frac{1 + (7 + 26a - 72b + 108c)r_j - (1 - 4a + 12b - 24c)r_j^2}{\prod^4_{\substack{i=1\\ i \neq j}} (1 - \frac{r_j}{r_i})},$$

j=1,2,3,4 and

$$\begin{aligned} W_4\mathbf{v}(t+l) &= \frac{l}{48}\left\{p_{17}(I-\frac{l}{r_1}A)^{-1}+p_{18}(I-\frac{l}{r_2}A)^{-1}+p_{19}(I-\frac{l}{r_3}A)^{-1}\right. \\ &+ \left. p_{20}(I-\frac{l}{r_4}A)^{-1}\right\}\mathbf{v}(t+l) \qquad (5.37) \end{aligned}$$

where

$$\begin{aligned} p_{16+j} &= \frac{1}{\prod_{\substack{i=1 \\ i\neq j}}^{4}(1-\frac{r_j}{r_i})}\{6+(44-168a+432b-648c)r_j \\ &+ (11-44a+132b-216c)r_j^2+(2-8a+24b-48c)r_j^3\}, \end{aligned}$$

j=1,2,3,4.

So

$$\begin{aligned} \mathbf{U}(t+l) &= A_1^{-1}\left[p_1\mathbf{U}(t)+\frac{l}{48}\{2p_5\mathbf{v}(t)+9p_9\mathbf{v}(t+\frac{l}{3})+18p_{13}\mathbf{v}(t+\frac{2l}{3})\right. \\ &+ \left. p_{17}\mathbf{v}(t+l)\}\right] \\ &+ A_2^{-1}\left[p_2\mathbf{U}(t)+\frac{l}{48}\{2p_6\mathbf{v}(t)+9p_{10}\mathbf{v}(t+\frac{l}{3})+18p_{14}\mathbf{v}(t+\frac{2l}{3})\right. \\ &+ \left. p_{18}\mathbf{v}(t+l)\}\right] \\ &+ A_3^{-1}\left[p_3\mathbf{U}(t)+\frac{l}{48}\{2p_7\mathbf{v}(t)+9p_{11}\mathbf{v}(t+\frac{l}{3})+18p_{15}\mathbf{v}(t+\frac{2l}{3})\right. \\ &+ \left. p_{19}\mathbf{v}(t+l)\}\right] \\ &+ A_4^{-1}\left[p_4\mathbf{U}(t)+\frac{l}{48}\{2p_8\mathbf{v}(t)+9p_{12}\mathbf{v}(t+\frac{l}{3})+18p_{16}\mathbf{v}(t+\frac{2l}{3})\right. \\ &+ \left. p_{20}\mathbf{v}(t+l)\}\right], \qquad (5.38) \end{aligned}$$

where

$$A_i = I-\frac{l}{r_i}A, \quad i=1,2,3,4. \qquad (5.39)$$

Hence

$$\mathbf{U}(t+l)=\mathbf{y}_1(t)+\mathbf{y}_2(t)+\mathbf{y}_3(t)+\mathbf{y}_4(t) \qquad (5.40)$$

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

$$\begin{aligned} A_1\mathbf{y}_1 &= p_1\mathbf{U}(t) + \frac{l}{48}\Big\{2p_5\mathbf{v}(t) + 9p_9\mathbf{v}(t+\frac{l}{3}) + 18p_{13}\mathbf{v}(t+\frac{2l}{3}) \\ &+ p_{17}\mathbf{v}(t+l)\Big\}, \qquad (5.41) \\ A_2\mathbf{y}_2 &= p_2\mathbf{U}(t) + \frac{l}{48}\Big\{2p_6\mathbf{v}(t) + 9p_{10}\mathbf{v}(t+\frac{l}{3}) + 18p_{14}\mathbf{v}(t+\frac{2l}{3}) \\ &+ p_{18}\mathbf{v}(t+l)\Big\}, \qquad (5.42) \\ A_3\mathbf{y}_3 &= p_3\mathbf{U}(t) + \frac{l}{48}\Big\{2p_7\mathbf{v}(t) + 9p_{11}\mathbf{v}(t+\frac{l}{3}) + 18p_{15}\mathbf{v}(t+\frac{2l}{3}) \\ &+ p_{19}\mathbf{v}(t+l)\Big\} \qquad (5.43) \\ A_4\mathbf{y}_4 &= p_4\mathbf{U}(t) + \frac{l}{48}\Big\{2p_8\mathbf{v}(t) + 9p_{12}\mathbf{v}(t+\frac{l}{3}) + 18p_{16}\mathbf{v}(t+\frac{2l}{3}) \\ &+ p_{20}\mathbf{v}(t+l)\Big\}, \qquad (5.44) \end{aligned}$$

respectively. For the purpose of implementation this algorithm is given in Table 5.1.

5.3 Numerical Examples

5.3.1 Example 1

Consider the problem {(4.41)–(4.44)} which is repeated here for convenience

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial t^2}, \quad 0 < x < 1, \quad t > 0. \qquad (5.45)$$

subject to the boundary conditions

$$\begin{aligned} u(0,t) &= 0, \quad t > 0, \qquad (5.46) \\ u(1,t) &= e^{-\frac{\pi^2}{4}t}, \quad t > 0, \qquad (5.47) \end{aligned}$$

and the initial condition

$$u(x,0) = sin(\frac{\pi}{2}x), \quad 0 \leq x \leq 1. \qquad (5.48)$$

Using the algorithm developed in Section 5.2 the problem {(5.45)–(5.48)} is solved for

$$h = 0.125, 0.1, 0.05, 0.025, 0.0125, 0.01, 0.005, 0.001$$

using

$$l = 0.125, 0.01, 0.05, 0.025, 0.0125, 0.01, 0.005, 0.001.$$

Only a representative numerical solution is depicted in Figure 5.1. 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 $t = 1.0$, are given with positions in Table 5.2.

In these experiments it is found that when both h and l are too small marvellous accuracy with very very small oscillations are obtained. For example, when $h = 0.002$ and $l = 0.0001$ the maximum error, at time $t = 1.0$, is $0.23302D-12$ at the position of $n = 271$. Moreover, accuracy can remarkably be increased for optimal values of h and l. For example, selecting $h = \frac{1}{202}$ and $l = 0.0002$ the maximum error obtained is $0.60174D - 13$ although the spatial and time steps are bigger. For this experiment maximum percentage relative error is $0.37104D - 09$.

5.3.2 Example 2

Consider the problem {(4.46)–(4.49)}, which is repeated here for convenience,

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial t^2}, \quad 0 < x < 1, \quad t > 0. \qquad (5.49)$$

subject to the boundary conditions

$$u(0,t) = t, \quad t > 0, \qquad (5.50)$$

$$u(1,t) = 0, \quad t > 0, \qquad (5.51)$$

and the initial condition

$$u(x,0) = 1, \quad 0 \le x \le 1. \tag{5. 52}$$

Using once again the algorithm developed in Section 5.2 the problem {(5.49)-(5.52)} is solved for

$$h = 0.125, 0.1, 0.05, 0.025, 0.01$$

with

$$l = 0.125, 0.1, 0.05, 0.025, 0.0125, 0.01.$$

Here also a representative numerical solution is depicted in Figure 5.2.

When these experiments are performed the similar observations to those in Chapter 4 were made, that is, when bigger values of h and l are used the method behaves smoothly over the whole interval $0 \le x \le 1$ but oscillations are observed for smaller values. The accuracy is also affected by smaller values of h and l because error grows rapidly near the end where the growing time-dependent boundary condition is given. Maximum errors, with positions, at time $t = 1.0$ are given in Table 5.4.

Table 5.1: Algorithm

Steps	Processor 1	Processor 2	Processor 3	Processor 4
1 Input	l, r_1, p_1 $p_5, p_9, p_{13},$ $p_{17}, \mathbf{U}_0, A$	$l, r_2, p_2,$ $p_6, p_{10}, p_{14},$ $p_{18}, \mathbf{U}_0, A$	$l, r_3, p_3,$ $p_7, p_{11}, p_{15},$ $p_{19}, \mathbf{U}_0, A$	$l, r_4, p_4,$ $p_8, p_{12}, p_{16},$ $p_{20}, \mathbf{U}_0, A$
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 Decomp	$I - \frac{l}{r_1}A$ $= L_1U_1$	$I - \frac{l}{r_2}A$ $= L_2U_2$	$I - \frac{l}{r_3}A$ $= L_3U_3$	$I - \frac{l}{r_4}A$ $= L_4U_4$
4 Evaluate	$\mathbf{v}_1, \mathbf{v}_2,$ $\mathbf{v}_3, \mathbf{v}_4,$	$\mathbf{v}_1, \mathbf{v}_2,$ $\mathbf{v}_3, \mathbf{v}_4,$	$\mathbf{v}_1, \mathbf{v}_2,$ $\mathbf{v}_3, \mathbf{v}_4,$	$\mathbf{v}_1, \mathbf{v}_2,$ $\mathbf{v}_3, \mathbf{v}_4,$
5 Using	$\mathbf{w}_1(t)$ $= 2p_5\mathbf{v}_1$ $+9p_9\mathbf{v}_2$ $+18p_{13}\mathbf{v}_3$ $+p_{17}\mathbf{v}_4$	$\mathbf{w}_2(t)$ $= 2p_6\mathbf{v}_1$ $+9p_{10}\mathbf{v}_2$ $+18p_{14}\mathbf{v}_3$ $+p_{18}\mathbf{v}_4$	$\mathbf{w}_3(t)$ $= 2p_7\mathbf{v}_1$ $+9p_{11}\mathbf{v}_2$ $+18p_{15}\mathbf{v}_3$ $+p_{19}\mathbf{v}_4$	$\mathbf{w}_4(t)$ $= 2p_8\mathbf{v}_1$ $+9p_{12}\mathbf{v}_2$ $+18p_{16}\mathbf{v}_3$ $+p_{20}\mathbf{v}_4$
6 Solve	$L_1U_1\mathbf{y}_1(t)$ $= p_1\mathbf{U}(t)$ $+\frac{l}{48}\mathbf{w}_1(t)$	$L_2U_2\mathbf{y}_2(t)$ $= p_2\mathbf{U}(t)$ $+\frac{l}{48}\mathbf{w}_2(t)$	$L_3U_3\mathbf{y}_3(t)$ $= p_3\mathbf{U}(t)$ $+\frac{l}{48}\mathbf{w}_3(t)$	$L_4U_4\mathbf{y}_4(t)$ $= p_4\mathbf{U}(t)$ $+\frac{l}{48}\mathbf{w}_4(t)$
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 $t = 1.0$

N	7	9	19	39
h	0.125	0.1	0.05	0.025
l=0.125	0.63647D-5 4	0.67172D-5 5	0.67753D-5 10	0.68054D-5 21
l=0.1	0.30403D-5 4	0.32927D-5 5	0.34603D-5 11	0.34756D-5 21
l=0.05	-0.90961D-7 1	0.20328D-6 6	0.36112D-6 11	0.37064D-6 22
l=0.025	-0.38877D-6 4	-0.13646D-6 5	0.22575D-7 12	0.31962D-7 23
l=0.0125	-0.41799D-6 4	-0.16568D-6 5	-0.77154D-8 10	0.18873D-8 26
l=0.01	-0.41934D-6 4	-0.16703D-6 5	-0.91071D-8 11	0.49143D-9 29
l=0.005	-0.42026D-6 4	-0.16795D-6 5	-0.10070D-7 11	-0.56061D-9 21
l=0.001	-0.42032D-6 4	-0.16801D-6 5	-0.10139D-7 11	-0.62958D-9 22

continued

Table 5.3: Continuation of Table 5.2

N	79	99	199	999
h	0.0125	0.01	0.005	0.001
l=0.125	0.68060D-5 42	0.68052D-5 52-53	0.68061D-5 105	0.68061D-4 524-526
l=0.1	0.34761D-5 42	0.34767D-5 53	0.34767D-5 106	0.34767D-5 529-532
l=0.05	0.37123D-6 44	0.37125D-6 55	0.37129D-6 111	0.37126D-6 552-555
l=0.025	0.32567D-7 47	0.32588D-7 59	0.32610D-7 117	0.32587D-7 585-586
l=0.0125	0.24547D-8 50	0.24775D-8 63	0.24961D-8 125	0.24706D-8 627
l=0.01	0.10290D-8 51	0.10519D-8 64	0.10685D-8 128	0.10234D-8 643
l=0.005	0.40063D-10 62	0.59368D-10 72	0.73882D-10 135-136	0.44144D-10 782-783
l=0.001	-0.40507D-10 44	-0.16193D-10 55	0.13386D-11 98	0.16917D-9 550-555

Positions are shown by space steps

Table 5.4: Maximum errors for Example 2 at the time t=1.0

N	7	9	19	39	99
h	0.125	0.1	0.05	0.025	0.01
l=0.125	0.1237D-4 4	0.1249D-4 5	0.1255D-4 10	0.1255D-4 20	0.1255D-4 50
l=0.1	0.6295D-5 4	0.6412D-5 5	0.6479D-5 10	0.6482D-5 20	0.6482D-5 50
l=0.05	0.5230D-6 4	0.6449D-6 5	0.7140D-6 10	0.7176D-6 20	-0.1161D-5 1
l=0.025	-0.1760D-6 2	0.1958D-6 1	-0.3831D-6 1	-0.3826D-6 2	-0.1181D-5 1
l=0.0125	-0.2150D-6 2	0.1788D-6 1	-0.3918D-6 1	-0.3912D-6 2	-0.1183D-5 1
l=0.01	-0.2169D-6 2	0.1780D-6 1	-0.3922D-6 1	-0.3916D-6 2	-0.1183D-5 1

Positions are shown by space steps

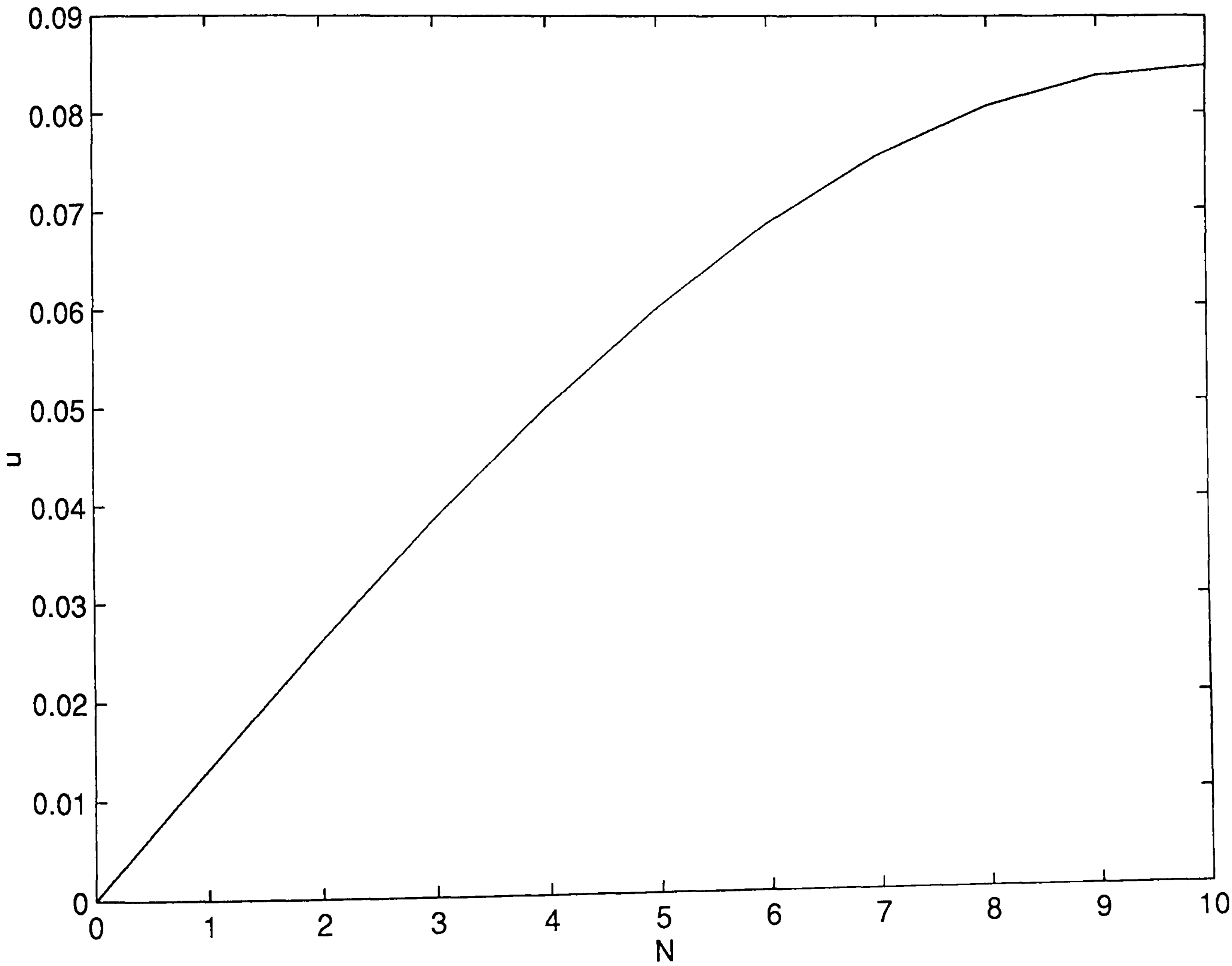

Figure 5.1: Numerical solution of numerical example 1 when h=0.1 and l=0.005 at time t=1.

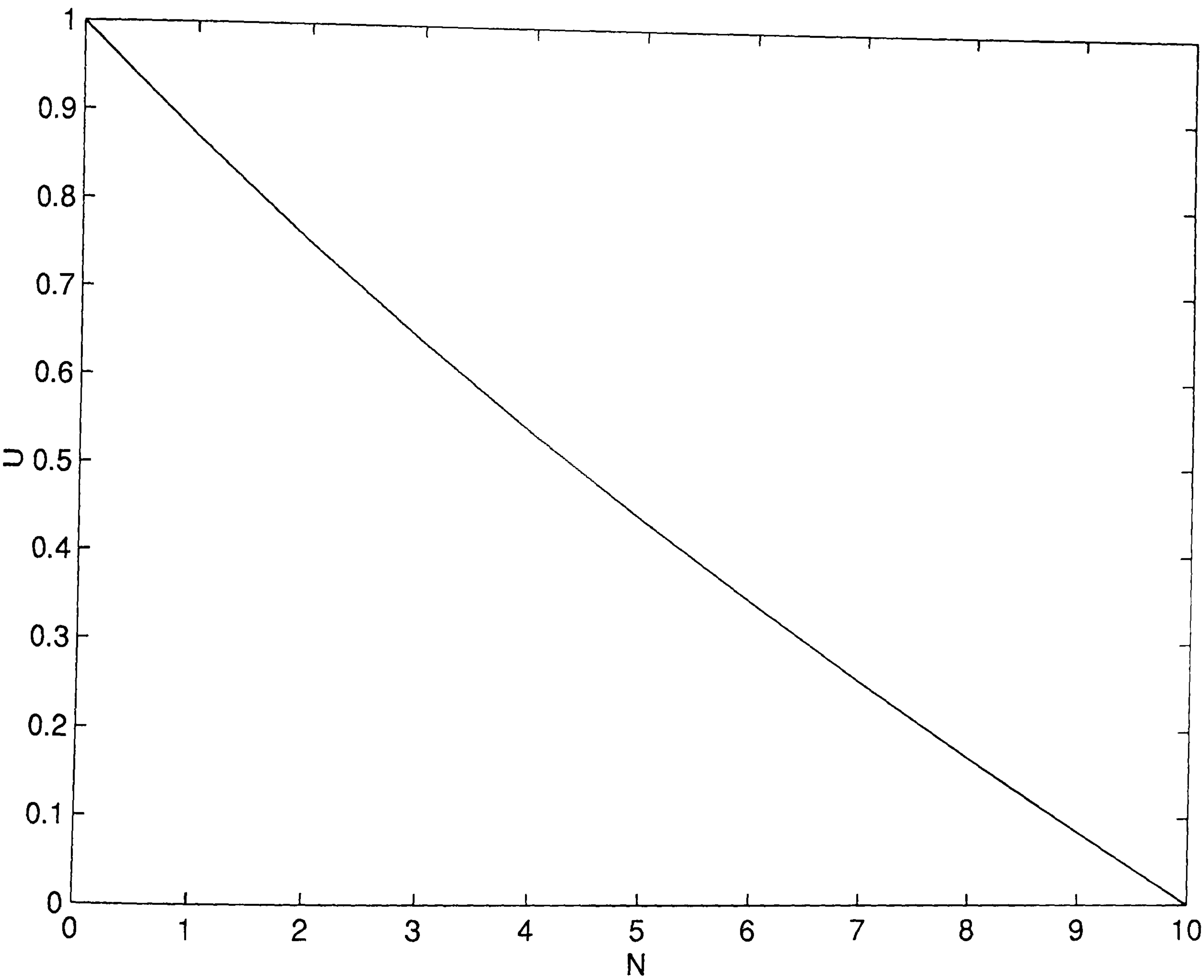

Figure 5.2: Numerical solution of numerical example 2 when h=0.1 and l=0.005 at time t=1.

Chapter 6

Summary and Conclusions

6.1 Summary

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

Chapter 1 was written for introductory purposes and covers some general topics, for example, basic introduction, motivation and aims of the thesis which are briefed in Sections 1.1 and 1.2 and some preliminaries which are needed in later chapters. For example, introduction of the method of lines, very important in solving parabolic partial differential equations, is given in Section 1.3, important notations are mentioned in Section 1.4, and some mathematical properties of finite-difference methods, for example, error analysis, consistency and stability, are outlined in Section 1.5.

In Chapter 2 a family of third-order numerical methods for one-dimensional heat equation, with constant coefficients, subject to the homogeneous boundary conditions, was introduced. Third-order accuracy in the space component is derived in Section 2.1 and a new governing matrix was obtained. In Section 2.2 the third-order acuuracy in the complementary component is obtained using a new rational approximation to the matrix exponential function, encountered in Section 2.1. Other relevant constraints for these methods are discussed in Sections 2.3 and 2.4. Since efficiency is also an important object of this thesis, a parallel algorithm which is implementable on architecture consisting of three processors is developed in Section 2.5. To make these methods more useful, extensions to two and three space dimensions with relevant algorithms are given in Sections 2.6 and 2.7 respectively. This chapter is concluded by numerical examples which show that the methods are very much effective. Pictorial evidence is also appended for support.

The matrix obtained in Chapter 2 is not symmetric so the maximum error, in some cases, is not at the centre of the region. To remove this rumple in error a family of fourth-order numerical methods for the one-dimensional heat equation, with constant coefficients, subject to homogeneous boundary conditions, is introduced in Chapter 3. Fourth-order accuracy in the space component is derived in Section 3.1 and a new quasi-symmetric matrix is obtained. In Section 3.2 a special case of the new rational approximation, given in Section 2.2, is suggested to achieve fourth-order accuracy in the time variable. Conditions for the L-stability of these methods are formulated in Sections 3.3. A parallel algorithm which is implementable on an architecture consisting of four processors is developed in Section 2.5. Like third-order methods these are also extended to two and three space dimensions in Sections 3.5 and 3.6 respectively. 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 and the maximum errors are at the centre of the region except in a few cases. Two numerical results are depicted for pictorial evidence.

There are many engineering problems in which the linear, homogeneous partial differential equation is given with time-dependent boundary conditions (Myers, 1971),for example, simple wall problem. So the Chapters 4 and 5 are intended to develop third- and fourth-order numerical methods for problems with time-dependent boundary conditions.

Considering a typical problem with time-dependent boundary conditions, a family of third-order numerical methods is developed in Chapter 4. Derivation of the methods is outlined in section 4.1 in which the matrix exponential function is approximated by the rational approximation introduced in section 2.2 of Chapter 2 and the quadrature term is approximated in a new way. 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 4.2, 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 4.3 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 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 3.2 and the quadrature term is approximated by a method which is an extended form of the method used in section 4.1. 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 problems given in Chapter 4. Using the aforesaid method extraordinary accuracy is achieved for one numerical example. Two numerical solutions are graphed and appended at the end of the chapter.

6.2 Applications

The ideas developed in this thesis can play an important rôle in modifying the methods for non-linear, first-order systems of ordinary differential equations which appear in the description of measels epidemiology, the dynamics of diabetology and population dynamics, linear parabolic partial differential equations with time-dependent source terms arising in the study of polymers and ceramics, linear or nonlinear parabolic partial differential equations with no source term arising in the study of percutaneous drug absorption, partial differential equations appearing in the diffusion in composite media (for example, heat in walls) and linear or nonlinear parabolic partial differential equations arising in the study of heat flow in the human body. In addition to parabolic partial differential equations these methods can be applied to second-order hyperbolic partial differential equations.

6.3 Conclusions

Up-to-now there was no direct method to achieve higher-order accuracy in the space variable. So the work considered in this thesis may be regarded as a first attempt in this direction and has revealed a lot of exciting observations.

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APPENDICES

Appendix A

Eigenvalues of h^2A given by (2.21)

Table A.1: Eigenvalues of h^2A for N=7

No.	Real Eigenvalues	No.	Complex Eigenvalues
1	-0.0987	5	-2.6893+0.5144i
2	-0.3944	6	-2.6893-0.5144i
3	-0.8933	7	-2.4685+0.2118i
4	-2.5359		

Table A.2: Eigenvalues of h^2A for N=9

No.	Real Eigenvalues	No.	Complex Eigenvalues
1	-0.0987	6	-2.6893+0.5144i
2	-0.3944	7	-2.6893-0.5144i
3	-0.8933	8	-2.4685+0.2118i
4	-1.5955	9	-2.4685-0.2118i
5	-2.5359		

Table A.3: Eigenvalues of h^2A for N=19

No.	Real Eigenvalues	No.	Complex Eigenvalues
1	-0.0247	10	-2.7066+0.6443i
2	-0.2217	11	-2.7066-0.6443i
3	-0.0987	12	-2.6607+0.5369i
4	-0.3932	13	-2.6607-0.5369i
5	-0.6124	14	-2.5925+0.3760i
6	-0.8775	15	-2.5925-0.3760i
7	-1.1842	16	-2.4975+0.2113i
8	-1.5259	17	-2.4975-0.2113i
9	-1.8977	18	-2.3747+0.0248i
		19	-2.3747-0.0248i

Table A.4: Eigenvalues of h^2A for N=39

No.	Real Eigenvalues	No.	Complex Eigenvalues
1	-0.0062	22	-2.7182 + 0.6729i
2	-0.0247	23	-2.7182 - 0.6729i
3	-0.0555	24	-2.7043 + 0.6480i
4	-0.0987	25	-2.7043 - 0.6480i
5	-0.1541	26	-2.6816 + 0.6066i
6	-0.2216	27	-2.6816 - 0.6066i
7	-0.3012	28	-2.6510 + 0.5495i
8	-0.3927	29	-2.6510 - 0.5495i
9	-0.4957	30	-2.6135 + 0.4776i
10	-0.6099	31	-2.6135 - 0.4776i
11	-0.7349	32	-2.5709 + 0.3935i
12	-0.8701	33	-2.5709 - 0.3935i
13	-1.0147	34	-2.5231 + 0.3031i
14	-1.1677	35	-2.5231 - 0.3031i
15	-1.3284	36	-2.4669 + 0.2137i
16	-1.4957	37	-2.4669 - 0.2137i
17	-1.6689	38	-2.4150 + 0.1201i
18	-1.8478	39	-2.4150 - 0.1201i
19	-2.0335		
20	-2.2324		
21	-2.3898		

Appendix B

Coefficients of $q(\theta)$, defined by (2.30)

Table B.1: Coefficients of $q(\theta)$, defined by (2.30).

a_1	a_2	a_3
3/2	193/300	3/50
7/5	46/75	2/25
139/100	185092/300000	277/3125
67/50	176476/300000	2123/25000
131/100	171379/300000	8293/100000
6544/5000	171181/300000	8287/100000
65431/50000	171151/300000	8286/100000
65430883/50000000	171150649/300000000	8286/100000
1.308617651	0.570502158833	0.082859999999692
1.308617650549908	0.57050215860798	0.082859999999692

Appendix C

Octadiagonal solver

Consider the linear system

$$Aw = b \tag{3. 1}$$

where A is an octadiagonal constant coefficient matrix

$$A = \begin{bmatrix} a5_1 & a6_1 & a7_1 & a8_1 & & & & & \bigcirc \\ a4_2 & a5_2 & a6_2 & a7_2 & a8_2 & & & & \\ a3_3 & a4_3 & a5_3 & a6_3 & a7_3 & a8_3 & & & \\ a2_4 & a3_4 & a4_4 & a5_4 & a6_4 & a7_4 & a8_4 & & \\ a1_5 & a2_5 & a3_5 & a4_5 & a5_5 & a6_5 & a7_5 & a8_5 & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ & & a1_{N-2} & a2_{N-2} & a3_{N-2} & a4_{N-2} & a5_{N-2} & a6_{N-2} & a7_{N-2} \\ & & & a1_{N-1} & a2_{N-1} & a3_{N-1} & a4_{N-1} & a5_{N-1} & a6_{N-1} \\ \bigcirc & & & & a1_N & a2_N & a3_N & a4_N & a5_N \end{bmatrix} \tag{3. 2}$$

$w = [w_1, w_2, \ldots, w_N]^T$, T denoting the transpose, to be determined and $b = [b_1, b_2, \ldots, b_N]^T$ is a given vector. The LU-decomposition of A may be carried out by factorizing it into two matrices L and U such that $A = LU$

where

$$L = \begin{bmatrix} 1 & & & & & & \bigcirc \\ l4_2 & 1 & & & & & \\ l3_3 & l4_3 & 1 & & & & \\ l2_4 & l3_4 & l4_4 & 1 & & & \\ l1_5 & l2_5 & l3_5 & l4_5 & 1 & & \\ & \ddots & \ddots & \ddots & & & \\ \bigcirc & & l1_N & l2_N & l3_N & l4_N & 1 \end{bmatrix}_{N\times N}$$

and

$$U = \begin{bmatrix} u1_1 & u2_1 & u3_1 & u4_1 & & & \bigcirc \\ & u1_2 & u2_2 & u3_2 & u4_2 & & \\ & & \ddots & \ddots & \ddots & \ddots & \\ & & & u1_{N-3} & u2_{N-3} & u3_{N-3} & u4_{N-3} \\ & & & & u1_{N-2} & u2_{N-2} & u3_{N-2} \\ & & & & & u1_{N-1} & u2_{N-1} \\ \bigcirc & & & & & & u1_N \end{bmatrix}_{N\times N}$$

To find the non zero entries of L and U we have the algorithm

$$\begin{array}{|lcl|} u4_i & = & a8_i \quad i = 1, 2, \ldots, N \\ u1_1 & = & a5_1 \\ u2_1 & = & a6_1 \\ u3_1 & = & a7_1 \\ l4_2 & = & a4_2/u1_1 \\ u1_2 & = & a5_2 - l4_2u2_1 \\ u2_2 & = & a6_2 - l4_2u3_1 \\ u3_2 & = & a7_2 - l4_2u4_1 \\ l3_3 & = & a3_3/u1_1 \\ l4_3 & = & (a4_3 - l3_3u2_1)/u1_2 \\ u1_3 & = & a5_3 - l3_3u3_1 - l4_3u2_2 \\ u2_3 & = & a6_3 - l3_3u4_1 - l4_3u3_2 \\ u3_3 & = & a7_3 - l4_3u4_2 \\ l2_4 & = & a2_4/u1_1 \\ l3_4 & = & (a3_4 - l2_4u2_1)/u1_2 \\ l4_4 & = & (a4_4 - l2_4u3_1 - l3_4u2_2)/u1_3 \\ u1_4 & = & a5_4 - l2_4u4_1 - l3_4u3_2 - l4_4u2_3 \\ u2_4 & = & a6_4 - l3_4u4_2 - l4_4u3_3 \\ u3_4 & = & a7_4 - l4_4u4_3 \\ u3_4 & = & a7_4 - l4_4u4_3 \quad \text{continued} \end{array}$$

$$
\begin{array}{rcl}
FOR\ i & = & 5,6,\ldots,N \\
l1_i & = & a1_i/u1_{i-4} \\
l2_i & = & (a2_i - l1_iu2_{i-4})/u1_{i-3} \\
l3_i & = & (a3_i - l1_iu3_{i-4} - l2_iu2_{i-3})/u1_{i-2} \\
l4_i & = & (a4_i - l1_iu4_{i-4} - l2_iu3_{i-3} - l3_iu2_{i-2})/u1_{i-1} \\
u1_i & = & a5_i - l2_iu4_{i-3} - l3_iu3_{i-2} - l4_iu2_{i-1} \\
u2_i & = & a6_i - l3_iu4_{i-2} - l4_iu3_{i-1} \\
u3_i & = & a7_i - l4_iu4_{i-1}
\end{array}
$$

Introducing an intermediate vector $\mathbf{x}$ we can write the given system as

$$U\mathbf{w} = \mathbf{x}, \qquad L\mathbf{x} = \mathbf{b}. \tag{3. 3}$$

We can solve these systems by forward and backward substitutions using the algorithms

$$
\begin{array}{rcl}
x_1 & = & b_1 \\
x_2 & = & b_2 - l4_2x_1 \\
x_3 & = & b_3 - l3_3x_1 - l4_3x_2 \\
x_4 & = & b_4 - l2_4x_1 - l3_4x_2 - l4_4x_3 \\
FOR\ i & = & 5,6,\ldots,N \\
x_i & = & b_i - l1_ix_{i-4} - l2_ix_{i-3} - l3_ix_{i-2} - l4_ix_{i-1}
\end{array}
$$

and

$$
\begin{array}{rcl}
w_N & = & x_N/u1_N \\
w_{N-1} & = & (x_{N-1} - u2_{N-1}w_N)/u1_{N-1} \\
w_{N-2} & = & (x_{N-2} - u2_{N-2}w_{N-1} - u3_{N-2}w_N)/u1_{N-2} \\
FOR\ i & = & N-3, N-4, \ldots, 1 \\
w_i & = & (x_i - u2_iw_{i+1} - u3_iw_{i+2} - u4_iw_{i+3})/u1_i
\end{array}
$$

respectively. This algorithm has a considerable advantage in CPU-time over the full Gauss elimination method.

Appendix D

Eigenvalues of h^2A given by (3.20)

Table D.1: Eigenvalues when N=7

No.	Real Eigenvalues	No.	Complex Eigenvalues
1	-4.0212	6	-2.5248+0.8053i
2	-0.1542	7	-2.5248-0.8053i
3	-0.6170		
4	-1.5412		
5	-2.6167		

Table D.2: Eigenvalues when N=9

No.	Eigenvalues	No.	Eigenvalues
1	-4.7966	6	-2.7934
2	-0.0987	7	-0.8963
3	-0.3941	8	-2.5209+0.6980i
4	-3.1892	9	-2.5209-0.6980i
5	-1.7899		

Table D.3: Eigenvalues when N=19

No.	Eigenvalues	No.	Eigenvalues
1	-5.2646	11	-1.6309
2	-5.0628	12	-1.2210
3	-4.7401	13	-0.8884
4	-4.3144	14	-2.1933
5	-3.8024	15	-0.6154
6	-3.1892	16	-2.5441+0.5221i
7	-0.0247	17	-2.5441-0.5221i
8	-0.0987	18	-2.6249+0.5006i
9	-0.2219	19	-2.6249+0.5006i
10	-0.3941		

Table D.4: Eigenvalues when N=39

No.	Eigenvalues	No.	Eigenvalues
1	-5.3202	21	-1.3862
2	-5.2811	22	-1.2055
3	-5.2165	23	-1.0385
4	-5.1271	24	-0.0062
5	-5.0140	25	-0.8847
6	-4.8787	26	-0.0247
7	-4.7225	27	-0.0555
8	-4.5474	28	-0.7436
9	-4.3551	29	-0.0987
10	-4.1475	30	-0.1542
11	-3.9264	31	-0.6149
12	-3.6931	32	-0.3941
13	-3.4480	33	-0.3019
14	-3.1892	34	-0.4984
15	-2.9087	35	-0.2219
16	-2.5937	36	-2.5794 + 0.5049i
17	-2.2859	37	-2.5794 - 0.5049i
18	-2.0242	38	-2.5794 + 0.5027i
19	-1.7928	39	-2.5794 -0.5027i
20	-1.5814		

Appendix E

Coefficients of $q(\theta)$, defined by (3.25)

Table E.1: Values of parameters for $q(\theta)$, defined by (3.25).

a_1	a_2	a_3
2.550	$2.338\dot{3}$	$0.9158\dot{3}$
2.558	$2.342\dot{3}$	0.9165
2.559	$2.3328\dot{3}$	$0.91158\dot{3}$
2.560	$2.33\dot{3}$	$0.911\dot{6}$
2.570	$2.358\dot{3}$	0.9225
2.580	$2.38\dot{3}$	$0.9\dot{3}$
2.590	$2.398\dot{3}$	$0.9391\dot{6}$
2.600	$2.42\dot{3}$	0.95
2.700	$2.58\dot{3}$	$1.02\dot{3}$
3.000	$3.09\dot{3}$	$1.258\dot{3}$