NUMERICAL SOLUTIONS OF DIFFUSION-TYPE EQUATIONS

A Dissertation

Presented to

the Faculty of the Department of Mechanical Engineering

University of Houston

In Partial Fulfillment

of the Requirements for the Degree

Doctor of Philosophy

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by

John Loyd Bryan

May, 1969

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ABSTRACT

A method of obtaining numerical solutions of a general class of boundary-value problems governed by the two-dimensional diffusion equation is investigated. The method employs a partial discretization of independent variables to reduce the problem of partial differential equations to a sequence of related boundary-value problems governed by a system of linear second-order ordinary differential equations. The generality of the method is demonstrated by applications to example problems involving both regular and irregular boundaries with boundary conditions of a general type. Application of separation of variables techniques to obtain closed-form solutions of a certain class of problems is presented and the results are used to indicate the accuracy of the method. An investigation into the stability characteristics of the resulting system of ordinary differential equations is also presented. It is concluded that the method appears to show promise as an easily implemented numerical method but that the full potential of the approach will not be realized until significant advances have been made in both computing hardware and software.

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CHAPTER I

INTRODUCTION

The solution of boundary-value problems governed by partial differential equations is of unquestionable importance in the physical sciences. Analytic solutions are generally obtainable only for a limited number of simple problems. Consequently, the use of high-speed digital computers has increased to the point where the computer can be considered a basic tool for obtaining numerical approximations to the solutions of the more complex problems which may be encountered in reality. An efficient and successful utilization of the computer for the solution of a specific problem, however, may be difficult to realize unless the investigator is well-versed in the application of the various numerical techniques which may be employed. For this reason, relatively simple techniques which may easily be employed for a broad class of equations, boundary conditions, and domains of interest are needed.

The most commonly used numerical technique for obtaining approximate solutions of problems governed by partial differential equations is the finite difference method involving the complete discretization of all independent and dependent variables appearing in the governing equation. A mesh or network of grid lines for the independent variables is constructed in some systematic manner over the domain of interest for a specific problem and the approximate solution is considered only at the nodes or intersections of the grid lines over the domain. The partial differential equation is approximated over the domain by a large-scale system of difference equations at each of the nodes. These difference equations are obtained by replacing the partial derivatives with finite difference quotients, due consideration being given to the boundary conditions at nodes on or near the boundary of the domain for specific problems. All finite difference schemes employ this general approach and differ primarily only in the manner with which the approximations to the derivatives are made and in the technique used to solve the resulting set of difference equations.

Unfortunately, these finite difference schemes are not universally applicable to all problems which may be encountered and require considerable programming effort when applied to problems involving even slightly irregular boundaries. In addition, certain limitations may be imposed on the relative magnitudes of the grid spacings for the independent variables due to considerations of consistency, convergence, and stability. It is recognized that the indiscriminant use of a particular difference scheme without at least some attempt at a stability and consistency analysis for a specific application may lead to completely nonsensical results[1]. However, an accurate stability analysis is often difficult, if not impossible, to perform for other than the simplest problems.

Other techniques which may be employed for solving boundary-value problems of partial differential equations involve a reduction or transformation of the original problem to a related system of simpler problems. Generally these transformation techniques can be applied only for regular boundaries and may require a considerable amount of preliminary mathematical manipulation before the numerical solution can be implemented. The reduction of a complex problem to a simple problem is desirable; however, the ease with which this reduction can be accomplished is of considerable importance when it comes to the application of the reduction process to specific problems.

A promising reduction technique has recently been applied to several problems governed by partial differential equations in two independent variables. This technique, called the straight line method in Russian literature [2], employs a partial discretization of the independent variables to approximate the partial differential equation with a system of ordinary differential equations. The discretization process retains the continuous character of one of the independent variables such that the conditions imposed on the original problem lead either to an initial-value problem or to a boundary-value problem of ordinary differential equations. Solution of the resulting problem yields approximations to the desired solution along a discrete set of continuous lines over the domain of interest. Sarmin and Chudov [3] point out that the utilization of a numerical integration scheme to solve the resulting problem actually introduces a discretization of the "continuous" independent variable such that the equations are solved as difference equations rather than differential equations. Consequently, stability aspects may enter into the use of the method of lines in a manner similar to that of the pure finite difference schemes.

This paper is concerned with the extension of this latter method, the method of lines, to the solution of problems governed by partial differential equations in three independent variables. Specifically, the linear parabolic equation of second order known as the two-dimensional diffusion or heat conduction equation

$$\frac{\partial^2\theta}{\partial x^2} + \frac{\partial^2\theta}{\partial y^2} = \frac{\partial\theta}{\partial t} \tag{1.1}$$

is considered over a finite region in the xy-plane for time $t > 0$. The boundary-value problem associated with (1.1) requires specification of an initial condition in time throughout the region as well as boundary conditions along the entire boundary of the region for time $t > 0$. The boundary conditions considered are of Dirichlet type, with the solution θ specified over the entire boundary, and of mixed type, with θ specified over a portion of the boundary and the normal derivative θ_n specified over the remaining portion of the boundary. The regions considered consist of a rectangular region of the xy-plane having two adjacent sides coincident with the coordinate axes and the irregular region formed by replacing one of the rectangular boundary lines with a line inclined to both coordinate axes.

The numerical approach taken in the solution of the resulting boundary-value problem of ordinary differential equations is the method of particular solutions as described by Luckinbill [4] who applied the same approach, i.e., the method of lines coupled with the method of particular solutions, to the one-dimensional diffusion equation, the Laplace equation, and the Poisson equation as concerns the nonlinear problem of identifying unknown parameters appearing in these equations. In the same paper, Luckinbill also illustrated the ease by which irregular boundaries can be handled with this approach. Boyd [5] used a slightly modified form of this approach to obtain approximate solutions of certain acoustic radiation problems governed by the scalar Helmholtz equation and was able to handle boundary conditions of mixed type having a linear combination of the solution and its normal derivative specified. The text by Berezin and Zhidkov [2] provides an extensive list of references to earlier Russian publications on the method of lines as well as presenting a comprehensive discussion on the method in general.

CHAPTER II

FORMULATION OF THE GENERAL PROBLEM

As an illustrative example of the type of boundary-value problem considered in general and the manner in which the method of lines is employed, consider the problem of determining a time-varying scalar field $\theta = \theta(x,y,t)$ over the rectangular region $0 \leq x \leq a$, $0 \leq y \leq b$ for time $t > 0$. The field is governed by the partial differential equation

$$\frac{\partial^2\theta}{\partial x^2} + \frac{\partial^2\theta}{\partial y^2} = \frac{\partial\theta}{\partial t}, \quad 0 \leq x \leq a, \quad 0 \leq y \leq b, \quad t > 0 \tag{2.1}$$

and is prescribed initially to be

$$\theta(x,y,0) = G(x,y), \quad 0 \leq x \leq a, \quad 0 \leq y \leq b \tag{2.2}$$

and, for time $t > 0$, the field is subject to a set of boundary conditions such as follows:

$$\theta(x,0,t) = f(x,t), \quad \theta(x,b,t) = g(x,t), \quad 0 \leq x \leq a \tag{2.3a}$$

$$\theta_x(0,y,t) = p(y,t), \quad \theta_x(a,y,t) = q(y,t), \quad 0 \leq y \leq b \tag{2.3b}$$

where the subscript notation has been employed in (2.3b) to denote the partial derivative with respect to the independent variable appearing as the subscript.

The method of lines is applied by considering only discrete time stages $t = t_k$, $k = 0,1,2,\ldots$, and discrete lines $y = y_i$, $i = 0,1,\ldots,N,N+1$, where N denotes the number of lines to be considered in the interval $0 < y < b$. The continuous character of the independent variable x is retained. Adopting a subscript-superscript notation to identify quantities along specific lines at specific time stages, respectively, the approximate solution along the ith line at the kth stage is denoted by φ_i^k

$$\varphi_i^k = \varphi_i^k(x) \approx \theta(x, y_i, t_k). \tag{2.4}$$

For a constant line spacing Δy,

$$\Delta y = \frac{b}{N+1}, \tag{2.5}$$

the second-order central difference approximation to the spatial derivative

$$\mathcal{E}^2\varphi_i^k = \frac{1}{\Delta y^2}\left[\varphi_{i+1}^k - 2\varphi_i^k + \varphi_{i-1}^k\right] \approx \theta_{yy}(x,y_i,t_k) \tag{2.6}$$

is used to replace this derivative in the partial differential equation (2.1) along all interior lines $1 \leq i \leq N$ at the kth time stage, $k > 0$. Similarly, the time derivative is replaced by the first-order backward difference approximation

$$\mathcal{D}\varphi_i^k = \frac{1}{t_k - t_{k-1}}\left[\varphi_i^k - \varphi_i^{k-1}\right] \approx \theta_t(x,y_i,t_k). \tag{2.7}$$

Utilizing the index notation of (2.4) for the prescribed initial condition (2.2) and boundary conditions (2.3) and the operational notation D = d/dx, the problem resulting from this application of the method of lines can be stated in the form of an infinite sequence of boundary-value problems of ordinary differential equations of the form

$$D^2\varphi_i^K + \varepsilon^2\varphi_i^K = \mathcal{D}\varphi_i^K, \quad 0 \le x \le a, \quad 1 \le i \le N \tag{2.8a}$$

$$D\varphi_i^K(0) = p_i^K, \qquad 1 \le i \le N \tag{2.8b}$$

$$D\varphi_i^K(a) = q_i^K, \qquad 1 \le i \le N \tag{2.8c}$$

for each time stage t_k, k = 1,2,..., subject to a set of supplementary conditions

$$\varphi_i^0(x) = G_i(x), \quad 0 \le x \le a, \quad 0 \le i \le N+1 \tag{2.9a}$$

$$\varphi_0^K(x) = f^K(x), \quad \varphi_{N+1}^K(x) = g^K(x), \quad 0 \le x \le a, \quad K > 0 \tag{2.9b}$$

arising from the initial condition (2.2) and the boundary conditions (2.3a), respectively.

The fact that there are infinitely many of the boundary-value problems (2.8) is of no consequence mathematically since the problems may be solved separately in succession for k = 1,2,3,... starting with the prescribed condition (2.9a) and using the results obtained for each stage k for the inhomogeneous term in $\mathcal{D}\phi_i^k$ for the next stage k + 1. From a numerical viewpoint, however, the boundary conditions at x = a will never be met exactly due to the finite arithmetic employed by the computer and the truncation error associated with the numerical technique used to solve the boundary-value problem (2.8) at each stage. The inhomogeneous character of the governing equations, coupled with the approximate nature of the solution at the various stages, could conceivably result in a situation where the numerical solutions converge to erroneous results over an extended number of time stages if sufficient care is not taken in the computations. The method of particular solutions appears to be ideally suited for this situation due to the iterative technique employed which contributes greatly to the control of round-off error in the necessary computations.

Briefly, the method of particular solutions may be described as a variation of the classical approach to the solution of linear multi-point boundary-value problems governed by an inhomogeneous system of first-order ordinary differential equations. The solution of the boundary-value problem is taken as a linear combination of numerically integrated solutions of initial-value problems governed by the inhomogeneous system instead of a linear combination of similar solutions of the corresponding homogeneous system augmented by a single solution of the inhomogeneous system.

Starting with an initial estimate of the unknown initial values, and forming a system of linearly independent initial values by perturbing the unknown initial values slightly, the resulting solutions of the initial value problems are of a more comparable order of magnitude at points where boundary conditions are prescribed than are the solutions using the usual approach. This in turn leads to more numerical significance in the determination of the unknown multipliers in the linear combination of solutions for the method of particular solutions. The method is applied in an iterative manner wherein the initial estimate of the unknown initial values are updated following each application until the solution generated from this set of initial values meets the prescribed set of boundary conditions within a specified tolerance, effectively reducing the effect of round-off error. The method is easier to program than the usual method due to the fact that the same governing equation is applicable to all solutions generated. A slight increase in computations results from the fact that the order of the matrix to be inverted in the determination of the multipliers is increased by one due to the use of particular solutions rather than complementary solutions.

The numerical integration scheme employed in the integration of the initial value problems is arbitrary although schemes of high-order accuracy are always desirable from the viewpoint of the computational time required for a specified accuracy. However, the dependence of the problem (2.8) on the solution at the previous time stage requires that the solution at each stage be stored in an easily retrievable manner for computation of the solution at the next stage. Programming considerations dictate that step-by-step integration schemes proceed with a constant step throughout the integration interval for all time stages. Finite computer high-speed memory limits the information which can be stored concerning the solution at the previous stage without sophisticated programming and the use of external storage devices which can increase the running time considerably. The step-by-step integration scheme employed in this investigation was a Runge-Kutta scheme of fourth-order accuracy. The evaluation of the derivative at the mid-point of each integration step as required by the Runge-Kutta algorithm used was based on a linear interpolation of the previous solution to obtain the corresponding mid-point values. Although this interpolation process undoubtedly introduces additional error into the integration process, the error appears to be less than the truncation error associated with the Runge-Kutta scheme for sufficiently smooth solutions and sufficiently small step size.

Another integration technique employed was a power series method of the form described by Doiron [6]. In this scheme, the solution at the previous stage can be stored in the form of coefficients of a power series expansion about one or more points in the integration interval. The stored coefficients can then be used in determining the coefficients of similar power series expansions for arbitrary initial values on the solution at the stage in question. The accuracy obtainable with power series techniques is practically unlimited, except by machine limitations, within the radius of convergence of the expansions; however, for slowly convergent expansions or for integration over intervals larger than the radius of convergence the necessity of using multiple centers of expansion in order to hold a high accuracy presents a programming problem. For the problems considered, the integration was able to step directly to the point $x = a$ with high accuracy.

CHAPTER III

MATHEMATICAL CONSIDERATIONS

Separation of variables provides a particularly convenient approach to the analytic solution of the exact boundary-value problem (2.1)-(2.3) when the boundary conditions (2.3) are prescribed to vanish identically and when the initial condition (2.2) is of a certain form. In this approach, the zero boundary conditions lead to the determination of a fundamental system of solutions in the form

$$\vartheta(x,y,t) = X(x)\,Y(y)\,T(t) \tag{3.1}$$

by means of which the solution of the given boundary-value problem can be established from consideration of the initial condition (2.2). In cases where the initial condition can be represented exactly by a finite combination of the solutions (3.1) at $t = 0$, the resulting solution will be in closed form.

An analogous approach to the solution of the problem resulting from the method of lines reduction is presented in the following sections of this chapter. Under similar circumstances, this approach will also lead to closed-form solutions which can be compared to the corresponding solutions of the exact problem to indicate the convergence of the approximate solution.

Since the integration of the system of ordinary differential equations (2.8a) is to be performed numerically, the stability characteristics of (2.8) are of paramount importance. Consequently, the final sections of this chapter are used to show investigations into these stability characteristics in order to predict the behavior of the numerical solutions in terms of the general solution of the system.

Analytic solution of the approximating problem

Consider the exact problem governed by Equation (2.1) and subject to the boundary conditions

$$\theta(x,0,t) = \theta(x,b,t) = \theta(0,y,t) = \theta(a,y,t) = 0 \qquad (3.2)$$

for time $t > 0$, with the prescribed initial condition

$$\theta(x,y,0) = \sin\frac{\pi x}{a} \sin\frac{\pi y}{b} \qquad (3.3)$$

The approximating problem governed by Equation (2.8a) is then subject to the boundary conditions

$$\varphi_i^{\kappa}(0) = \varphi_i^{\kappa}(a) = 0, \quad 1 \le i \le N, \quad \kappa > 0 \qquad (3.4)$$

with the supplementary conditions

$$\varphi_0^{\kappa}(x) = \varphi_{N+1}^{\kappa}(x) = 0, \quad 0 \le x \le a, \quad \kappa > 0 \qquad (3.5a)$$

$$\varphi_i^{0}(x) = \sin\frac{\pi y_i}{b} \sin\frac{\pi x}{a}, \quad 0 \le x \le a, \quad 1 \le i \le N \qquad (3.5b)$$

The solution $\varphi_i^K(x)$ is assumed to consist of a linear combination of solutions of the form

$$\phi(x,i,k) = f(x)\,\alpha(i)\,\beta(k) \tag{3.6}$$

where

$$\begin{aligned} f(0) &= f(a) = 0 \\ \alpha(0) &= \alpha(N+1) = 0 \end{aligned} \tag{3.7}$$

such that the conditions (3.4) and (3.5a) are identically satisfied. The problem then reduces to the determination of allowable values of two unknown constant parameters ζ and η such that the second-order equations

$$\left[D^2 - \zeta\right] f(x) = 0 \tag{3.8a}$$

$$\left[E^2 - (2+\eta)E + 1\right]\alpha(i) = 0 \tag{3.8b}$$

possess non-trivial solutions $f(x)$ and $\alpha(i)$ satisfying the conditions (3.7). The notation E in Equation (3.8b) refers to the translational difference operator

$$E^n \alpha(i) = \alpha(i+n), \quad n = 1,2,3,\ldots \tag{3.9}$$

The solutions of the Sturm-Liouville systems (3.7) and (3.8) are found to be

$$f_m(x) = \sin\frac{m\pi x}{a}, \qquad \zeta_m = -\frac{m^2\pi^2}{a^2}, \quad m = 1,2,3,\ldots$$
$$\alpha_n(i) = \sin\frac{n\pi y_i}{b}, \qquad \eta_n = -2\left(1-\cos\frac{n\pi}{N+1}\right), \quad 1 \le n \le N. \tag{3.10}$$

For appropriate values of m and n, the first-order difference equation for $\beta(k)$,

$$\left[E - \frac{1}{1+\nu}\right]\beta(k) = 0,$$

where (3.11)

$$\nu = -\left[\zeta + \frac{\eta}{\Delta y^2}\right]\Delta t,$$

has the general solution

$$\beta_{mn}(k) = \frac{C_{mn}}{(1+\nu_{mn})^{k}} \tag{3.12}$$

where C_{mn} is an arbitrary constant and ν_{mn} is as defined in (3.10)-(3.11). The fundamental system of solutions thus consists of

$$\phi_{mn}(x,i,k) = \sin\frac{m\pi x}{a}\,\sin\frac{n\pi y_i}{b}\left(1+\nu_{mn}\right)^{-k} \tag{3.13}$$

where

$$\nu_{mn} = \frac{m^2\pi^2}{a^2} + \frac{2(1-\cos\frac{n\pi}{N+1})}{\Delta y^2} \quad \Delta t \tag{3.14}$$

for m = 1,2,3,... and n = 1,2,...,N.

It is apparent that the solution of the boundary-value problem subject to the initial condition (3.5b) is given by the single term for m = n = 1, i.e.,

$$\varphi_i^k(x) = \frac{\sin\frac{\pi x}{a} \quad \sin\frac{\pi y_i}{b}}{\left\{1 + \left[\frac{\pi^2}{a^2} + \frac{2(1-\cos\frac{\pi\Delta y}{b})}{\Delta y^2}\right]\Delta t\right\}^k} \tag{3.15}$$

for k = 0,1,2,... and $1 \le i \le N$. For comparison purposes, the closed-form solution of the exact problem along the ith line and at the kth time stage is given by

$$\theta(x,y_i,t_k) = \sin\frac{\pi x}{a} \sin\frac{\pi y_i}{b} \; e^{-\left(\frac{\pi^2}{a^2}+\frac{\pi^2}{b^2}\right)k\Delta t} \tag{3.16}$$

Defining the quantities

$$\nu^* = \frac{\pi^2}{a^2} + \frac{\pi^2}{b^2}$$

$$\nu = \frac{\pi^2}{a^2} + \frac{2(1-\cos\frac{\pi\Delta y}{b})}{\Delta y^2}, \tag{3.17}$$

and noting that

$$\lim_{\Delta y \to 0} \left[\frac{2(1 - \cos \frac{\pi \Delta y}{b})}{\Delta y^2} \right] = \frac{\pi^2}{b^2} \tag{3.18}$$

it can be concluded that ν approaches ν^* asymptotically as Δy decreases and is confined to the relatively small interval

$$\frac{\pi^2}{a^2} + \frac{\delta}{b^2} \leq \nu \leq \frac{\pi^2}{a^2} + \frac{\pi^2}{b^2} \tag{3.19}$$

Consequently, for sufficiently small Δt, the binomial expansion

$$(1 + \nu \Delta t)^{-K} = 1 - K\nu\Delta t + \frac{K(K+1)}{2!}(\nu\Delta t)^2 - \ldots \tag{3.20}$$

is valid for all k = 1,2,3,... . Comparing the expansion (3.20) with the expansion of the exponential term in (3.16),

$$e^{-K\nu^*\Delta t} = 1 - K\nu^*\Delta t + \frac{K^2}{2!}(\nu^*\Delta t)^2 - \ldots \tag{3.21}$$

the convergence of the approximate solution (3.15) to the exact solution (3.16) in the limit as Δt and Δy both approach zero is evident.

General solution of the approximating system

The fact that the analytical solution of the approximating problem converges to the exact solution may be of little or no consequence when the solution is attempted numerically due to the introduction of error in the computations. The successful application of the method of particular solutions requires that the boundary conditions at x = a be met within a small tolerance. In order that this tolerance can be held, the system of ordinary differential equations must be stable to the extent that any trend toward instability in the integration process can be controlled effectively by varying the initial values at x = 0 on each of the N lines. In order to study the stability of the system, it is sufficient to study the general solution of the system.

The system of Equation (2.8a) can be written using matrix notation in the form

$$\frac{d\vec{z}}{dx} = A\vec{z} + \vec{F} \tag{3.22}$$

where $\vec{z}=\vec{z}(x)$ is the state-variable vector having the 2N elements

$$z_i = \varphi_i^K, \quad z_{i+N} = D\varphi_i^K, \qquad i=1,2,\dots,N \tag{3.23}$$

and where the 2N x 1 vector $\vec{F}=\vec{F}(x)$ has the elements

$$f_i = 0, \quad f_{i+N} = -\frac{1}{\Delta t}\varphi_i^{K-1}, \quad i = 1,2,\ldots,N. \tag{3.24}$$

The 2N x 2N matrix A can be written in partitioned form as

$$A = \begin{bmatrix} O & I \\ S & O \end{bmatrix} \tag{3.25}$$

where O and I denote the N x N null and identity matrices, respectively, and S is the N x N tridiagonal matrix

$$S = \begin{bmatrix} \gamma & -\mu & & & \\ -\mu & \gamma & -\mu & & \\ & \ddots & \ddots & \ddots & \\ & & -\mu & \gamma & -\mu \\ & & & -\mu & \gamma \end{bmatrix} \tag{3.26}$$

with the non-zero terms $\mu = 1/\Delta y^2$, $\gamma = 2\mu + 1/\Delta t$.

The general solution of (3.22) can be written immediately in terms of complementary and particular solutions in the form

$$\vec{z}(x) = e^{Ax}\vec{C} + \vec{P}(x) \tag{3.27}$$

where $\vec{C}$ is a vector of 2N arbitrary constants, e^{Ax} is the matrix exponential of A, and $\vec{P}(x)$ is an arbitrary particular solution of the inhomogeneous system. The general form of the matrix exponential is difficult to ascertain; however, certain conclusions concerning the complementary solution can be made based on the 2N eigenvalues of A.

The eigenvalues of A can be determined from the N eigenvalues of the symmetric matrix S. Certain conclusions concerning the eigenvectors of A can also be reached from consideration of the eigenvectors of S. To illustrate, let S have the N real eigenvalues ξ_i and the N associated linearly independent eigenvectors $\vec{e}_i$ such that

$$S\vec{e}_i = \xi_i \vec{e}_i , \qquad i = 1, 2, \ldots, N \tag{3.28}$$

Retaining the partitioning of (3.25), the eigenvalue problem for A can be written as

$$\begin{bmatrix} 0 & I \\ S & 0 \end{bmatrix} \begin{Bmatrix} \vec{u} \\ \vec{v} \end{Bmatrix} = \lambda \begin{Bmatrix} \vec{u} \\ \vec{v} \end{Bmatrix} \tag{3.29}$$

where $\vec{u}$ and $\vec{v}$ are N x 1 vectors forming an eigenvector $\vec{w}$ of A associated with the eigenvalue λ. Carrying out the indicated matrix multiplications, the "shifted eigenvalue problem" [7] is obtained

$$\begin{aligned} I\vec{v} &= \lambda \vec{u} \\ S\vec{u} &= \lambda \vec{v} \end{aligned} \tag{3.30}$$

from which it follows that

$$\vec{v} = \lambda \vec{u}, \qquad S\vec{u} = \lambda^2 \vec{u}. \tag{3.31}$$

Consequently it is seen that the eigenvalues and eigenvectors of A are given by

$$\left.\begin{aligned} \lambda_i &= \xi_i^{1/2}, & \lambda_{i+N} &= -\lambda_i \\ \vec{w}_i &= \begin{Bmatrix} \vec{e}_i \\ \lambda_i \vec{e}_i \end{Bmatrix}, & \vec{w}_{i+N} &= \begin{Bmatrix} \vec{e}_i \\ -\lambda_i \vec{e}_i \end{Bmatrix} \end{aligned}\right\} i=1,2,\ldots,N \tag{3.32}$$

The eigenvalues λ_i of A will all be real since the eigenvalues ξ_i of S are positive owing to the strict diagonal dominance of S

$$|s_{ii}| > \sum_{j\neq i} |s_{ij}|, \quad i=1,2,\ldots,N \tag{3.33}$$

Furthermore, the N eigenvalues of S can be determined in explicit form as

$$\xi_i = \frac{2\left(1 - \cos \frac{i\pi}{N+1}\right)}{\Delta y^2} + \frac{1}{\Delta t}, \quad i=1,2,\ldots,N \tag{3.34}$$

indicating that both S and A have distinct eigenvalues.

Since the eigenvalues of A are distinct, the 2N eigenvectors $\vec{w}_i$ will be linearly independent. Consequently, the general solution (3.27) can be written

$$\vec{z}(x) = \sum_{i=1}^{N} \left\{ c_i e^{\lambda_i x} \vec{w}_i + c_{i+N} e^{-\lambda_i x} \vec{w}_{i+N} \right\} + \vec{P}(x) \tag{3.35}$$

where the c_i are arbitrary constants, and where the eigenvalues $\lambda_i > 0$ are

$$\lambda_i = \left\{ \frac{4}{\Delta y^2} \sin^2 \frac{i\pi}{2(N+1)} + \frac{1}{\Delta t} \right\}^{1/2}, \quad i = 1, 2, \ldots, N \tag{3.36}$$

Owing to the presence of the positive exponentials in the general solution, the system is seen to be unstable in the sense that all solutions of the homogeneous equation do not approach zero as x increases. However, solutions which are strictly stable are theoretically possible [8]. The numerical integration of the equations can be expected to present difficulties since the numerical solution will in general contain components of each of the exponential terms. This instability can be expected to increase with a reduction in the time step Δt or, to a certain extent, a reduction in the line spacing Δy. This presents somewhat of a dilemma since the first-order approximation for the time derivative implies the necessity of a very small time step for acceptable accuracy. The integration interval may prohibit numerical solution for even large time steps. One conclusion is obvious, a high degree of accuracy is essential in the numerical integration.

CHAPTER IV

NUMERICAL EXAMPLES AND DISCUSSION OF RESULTS

The unstable character of the system of ordinary differential equations (2.8a) arising from the method of lines does not necessarily invalidate the numerical solution of the related boundary-value problems. However, a certain amount of difficulty in obtaining usable solutions can be expected, especially if the time increment Δt is chosen small in an attempt to improve the accuracy of the approximation. The integration interval and the line spacing Δy can also be expected to influence the success or failure of the method for specific problems.

In order to subject the method to a numerical test three example problems were considered. A series of numerical experiments was conducted using these examples in order to obtain information relating to the effect of line spacing, time increment, integration scheme, and the length of the integration interval. Due to the critical nature of the solution at the first time stage, attention was directed primarily toward obtaining usable solutions at the first time stage. The example problems and the results of the numerical experimentation are presented in the following sections of this chapter. All computations, unless otherwise specified, were performed in double precision floatingpoint arithmetic using an IBM 360/44 computer capable of carrying approximately sixteen significant figures.

A mixed problem in a rectangle

The first subject of the numerical experimentation was a problem over a rectangular region of the xy-plane in which the boundary conditions were imposed on both the solution and the normal derivative. Specifically, the exact problem which was considered is described by the governing partial differential equation (2.1) and boundary conditions of the type indicated in (2.3) with

$$\begin{aligned} f(x,t) &= g(x,t) = 0, \quad 0 \leq x \leq a, \quad t > 0 \\ p(y,t) &= q(y,t) = 0, \quad 0 \leq y \leq b, \quad t > 0 \end{aligned} \qquad (4.1)$$

The dimensions of the rectangle were taken as $a = b = 1$ and the initial condition (2.2) was prescribed by

$$G(x,y) = \sin \pi y \,(1 + \cos \pi x) \qquad (4.2)$$

The analytic solution of this problem by separation of variables yields the closed-form result

$$\theta(x,y,t) = \sin \pi y \left(e^{-\pi^2 t} + e^{-2\pi^2 t} \cos \pi x \right) , \qquad (4.3)$$

Application of the method of lines reduction resulted in a sequence of related boundary-value problems governed by the system of ordinary differential equations (2.8a). The solution of this system at successive time stages k = 1,2,3,... was subject to the boundary conditions

$$D\varphi_i^k(0) = D\varphi_i^k(1) = 0, \quad 1 \le i \le N. \tag{4.4}$$

The supplementary conditions (2.9) became

$$\begin{aligned} \varphi_i^0(x) &= \sin\frac{i\pi}{N+1}\left(1 + \cos\pi x\right), \quad 1 \le i \le N, \quad 0 \le x \le 1 \\ \varphi_0^k(x) &= \varphi_{N+1}^k(x) = 0, \quad k > 0, \quad 0 \le x \le 1 \end{aligned} \tag{4.5}$$

The separation of variables approach discussed in Chapter III led to the closed-form solution

$$\varphi_i^k(x) = \sin\frac{i\pi}{N+1}\left\{\frac{1}{(1+\nu_{01}\Delta t)^k} + \frac{\cos\pi x}{(1+\nu_{11}\Delta t)^k}\right\} \tag{4.6}$$

where ν_{01} and ν_{11} are as defined by Equation (3.14) for appropriate values of m and n.

The convergence of the approximate solution (4.6) to the exact solution (4.3) at the first time stage as the line spacing and time increment approach zero is indicated for the points x = 0, y = 0.5 and x = 1, y = 0.5 in Tables 4.1 and 4.2, respectively. It can be seen that the approximate

TABLE 4.1

CONVERGENCE OF THE APPROXIMATE SOLUTION
TO THE EXACT SOLUTION AT $x = 0$, $y = 0.5$
FOR THE MIXED PROBLEM

TIME STEP Δt	APPROXIMATE SOLUTION				EXACT SOLUTION
	Line spacing Δy				
	1/2	1/4	1/8	1/16	
1	.16411	.14581	.14159	.14056	.00005
1/2	.30066	.27001	.26284	.26108	.00724
1/4	.51624	.47122	.46045	.45778	.09200
1/8	.80924	.75416	.74059	.73721	.37602
1/16	1.13907	1.08460	1.07079	1.06733	.83085
1/32	1.44167	1.39794	1.38659	1.38372	1.27424
1/64	1.67062	1.64110	1.63331	1.63133	1.59169
1/128	1.81867	1.80109	1.79640	1.79520	1.78288
1/256	1.90445	1.89477	1.89217	1.89151	1.88797
1/512	1.95089	1.94580	1.94443	1.94408	1.94309
1/1024	1.97510	1.97249	1.97178	1.97160	1.97132

TABLE 4.2

CONVERGENCE OF THE APPROXIMATE SOLUTION
TO THE EXACT SOLUTION AT $x=1$, $y=0.5$
FOR THE MIXED PROBLEM

TIME STEP Δt	APPROXIMATE SOLUTION Line spacing Δy 1/2	1/4	1/8	1/16	EXACT SOLUTION
1	.05812	.04701	.04457	.04398	.00005
1/2	.09934	.08171	.07777	.07681	.00714
1/4	.15043	.12702	.12165	.12034	.07761
1/8	.19076	.16683	.16115	.15975	.20641
1/16	.19427	.17660	.17224	.17116	.24843
1/32	.15833	.14897	.14659	.14599	.19496
1/64	.10716	.10342	.10244	.10220	.12249
1/128	.06368	.06246	.06213	.06205	.06870
1/256	.03495	.03459	.03450	.03447	.03639
1/512	.01834	.01824	.01822	.01821	.01873
1/1024	.00940	.00937	.00937	.00937	.00950

solution for each time increment appears to approach a limiting value as the line spacing is successively halved and that this limiting value approaches the exact solution as the time increment is successively halved.

The behavior of the approximate solution as shown in Tables 4.1 and 4.2 clearly indicates the necessity of a small time increment for an accurate approximation. However, the analysis of Chapter III indicated that the system of equations (2.8a) will become more and more unstable as the time increment is reduced whereas the effect caused by reducing the line spacing will not be as pronounced. Consequently, the first numerical experiment was directed toward further investigation into the stability of the numerical integration of Equations (2.8a). The equations were integrated numerically using a constant step fourth-order Runge-Kutta scheme and a power series scheme over the interval $0 \leq x \leq 1$ from initial values obtained from the closed-form solution (4.6). Table 4.3 presents the results of this stability test for the case of a 9-line approximation ($\Delta y = 0.1$). The tabulated values are the resulting solution value at $x = 1$ for the central line $y = 0.5$. The analytic solutions at the same point are included for purposes of comparison. Runs for other line spacings showed similar results. For this series of stability tests, the forcing function arising from the initial condition (4.5a) was defined analytically

TABLE 4.3

RESULTS OF 9-LINE APPROXIMATION STABILITY TEST FOR THE MIXED PROBLEM

TIME STEP Δt	INTEGRATION RESULTS AT $x=1$, $y=0.5$ — fourth-order RUNGE-KUTTA, step size h: 1.E-01	1.E-02	5.E-03	1.E-03	1.E-04	POWER SERIES	ANALYTIC SOLUTIONS: Approx.	Exact
1	.04431	.04428	--*	--	--	--	.04428	.00005
1/2	.07738	.07731	--	--	--	--	.07731	.00714
1/4	.12123	.12102	--	--	--	--	.12102	.07761
1/8	.16132	.16048	--	--	--	--	.16048	.20641
1/16	.17669	.17172	--	--	--	--	.17172	.24843
1/32	.19368	.14631	.14630	--	--	--	.14630	.19496
1/64	.94822	.10245	.10233	.10232	--	--	.10232	.12249
1/128	4.E+01	.06865	.06251	.06210	--	--	.06209	.06870
1/256	5.E+03	1.E 00	.12131	.03466	.03455	.03449	.03449	.03639
1/512	3.E+06	2.E+03	1.E+02	.22608	.02140	.01842	.01822	.01873
1/1024	7.E+09	4.E+07	3.E+06	5.E+03	3.E 00	.34442	.00937	.00950

* Value agrees with value on the left through at least the fifth decimal place.

to avoid the introduction of additional error through the interpolation process which otherwise would have been required by the Runge-Kutta algorithm and to permit the power series scheme to utilize subsequent points of expansion in the integration interval as required. The results shown clearly indicate the effect of the time increment on the stability of the Runge-Kutta integration and the increased accuracy obtainable by the power series scheme.

In general, the power series integration scheme was able to step directly to the point $x = 1$ using the single expansion about $x = 0$. This was not possible for the two smallest time steps considered; however, it was noticed that the end results using these multiple expansions did not differ appreciably from the results using a single point of expansion. Consequently, it was decided to incorporate a single-expansion power series scheme for subsequent runs. This not only simplified the programming of the power series scheme for use in solving the boundary-value problems but also reduced the computational time and storage requirements considerably as well as leading to a more stable and accurate scheme. Explicit time comparisons are not available; however, the computational time required for the power series integration using a maximum of fifty terms in the expansions was comparable to the time required for the Runge-Kutta scheme with step size $h = 0.1$ while yielding accuracy comparable to the much slower Runge-Kutta scheme with integration step size $h = 0.0001$. Needless to say, this smaller Runge-Kutta integration step is not suited for numerical solution of the boundary-value problems due to the amount of computer memory required.

The next numerical experiment was designed to test the ability of the method of particular solutions to correctly determine the solution values at $x = 0$ such that the zero boundary conditions on the derivative at $x = 1$ were satisfied within a reasonable tolerance. The results of this experiment, again for the 9-line approximation, are given in Table 4.4. The tabulated values include the final solution values along the center line $y = 0.5$ at the ends of the integration interval and the average order of magnitude of the derivatives at $x = 1$. The values of the closed-form solution at $x = 0$ and $x = 1$ are also given for comparison. The computed values at $x = 0$ are shown only to five decimal places; however, the agreement with the analytic solution was almost exact in all cases, differing only in the fifteenth or sixteenth significant figures.

In order to determine whether or not the fact that the solution at $x = 1$ approached zero as the time increment approached zero had any bearing on the loss of accuracy for the smaller time steps, the integration was performed in the reverse direction. The results of this run for the 9-line

TABLE 4.4

MIXED BOUNDARY-VALUE PROBLEM RESULTS
FOR A 9-LINE APPROXIMATION

TIME STEP Δt	SOLUTION VALUES FOR $y = 0.5$ COMPUTED $x = 0$	COMPUTED $x = 1$	ANALYTIC $x = 0$	ANALYTIC $x = 1$	AVERAGE ERROR AT $x = 1$*
1	.14110	.04428	.14110	.04428	1.E-08
1/4	.45917	.12102	.45917	.12102	1.E-08
1/16	1.06913	.17172	1.06913	.17172	1.E-08
1/64	1.63236	.10232	1.63236	.10232	1.E-06
1/256	1.89186	.03449	1.89186	.03449	1.E-05
1/1024	1.97170	-.44875	1.97170	.00937	1.E+01

* Average order of magnitude of computed derivative over all lines.

TABLE 4.5

MIXED BOUNDARY-VALUE PROBLEM RESULTS
FOR A 9-LINE APPROXIMATION WITH REVERSE INTEGRATION

TIME STEP Δt	COMPUTED SOLUTION FOR $y = 0.5$ $x = 0$	$x = 1$	AVERAGE ERROR AT $x = 0$*
1	.14110	.04428	1.E-10
1/4	.45917	.12102	1.E-09
1/16	1.06913	.17172	1.E-08
1/64	1.63236	.10232	1.E-08
1/256	1.89186	.03449	1.E-07
1/1024	1.96937	.00937	1.E-02

* Average order of magnitude of computed derivative over all lines.

approximation are presented in Table 4.5. The results do show a higher accuracy although five decimal accuracy still could not be obtained for the smallest time step.

A Dirichlet problem in a rectangle

The next subject of the numerical experimentation was a problem over a rectangular region of the xy-plane for which boundary conditions were imposed only on the solution. Specifically, the problem considered was the example for which closed-form solutions were obtained in Chapter III. The problem was described by Equations (2.1), (3.2), and (3.3) and had the approximate and exact closed-form solutions (3.15) and (3.16), respectively. Verification of the remarks made concerning the convergence of the approximate solution (3.15) to the exact solution (3.16) as the time increment and line spacing approach zero is given by Table 4.6. The values given are for the solution at the midpoint of the unit square, $a = b = 1$.

The first numerical experiment conducted on this problem was designed to investigate the ability of the method of particular solutions to produce meaningful solutions of the resulting boundary value problems over the unit square $a = b = 1$ as the line spacing and time increment were varied. Items of interest in this investigation included the resulting solution values at $x = 1$ for comparison with the zero

TABLE 4.6

CONVERGENCE OF THE APPROXIMATE SOLUTION
TO THE EXACT SOLUTION AT THE MIDPOINT
OF A UNIT SQUARE FOR THE DIRICHLET PROBLEM

TIME STEP Δt	APPROXIMATE SOLUTION, Line spacing Δy: 1/2	1/4	1/8	1/16	EXACT SOLUTION
1/2	.10066	.09415	.09254	.09213	.00005
1/4	.18290	.17210	.16940	.16872	.00719
1/8	.30924	.29366	.28972	.28873	.08481
1/16	.47240	.45400	.44927	.44809	.29121
1/32	.64167	.62449	.62000	.61887	.53964
1/64	.78173	.76884	.76543	.76457	.73460
1/128	.87750	.86932	.86713	.86658	.85709
1/256	.93475	.93009	.92884	.92852	.92579
1/512	.96628	.96378	.96311	.96294	.96218
1/1024	.98285	.98156	.98121	.98112	.98091

boundary conditions imposed, the resulting solution at the midpoint of the integration interval, and the derivative along the lines at the midpoint of the integration interval. These quantities are given in Table 4.7 for the case of a 9-line approximation. The symmetry of this problem was incorporated for an alternate approach to the solution by considering only half of the unit square with zero boundary conditions imposed on the derivative at $x = 0.5$. The results for this approach did not differ from those of the original formulation; however, the imposed boundary conditions on the derivative were satisfactorily met using this approach. The results of this last test indicated that the integration interval can contribute considerably to the stability of the numerical solution.

To obtain additional indication of the effect produced by changes in the integration interval, the value of the end point $x = a$ was varied over the range $0.6 \leq a \leq 1.5$ for various time steps. The results presented in Table 4.8 for this test indicate the dependency of the stability of the numerical integration on the integration interval for a time increment of 0.001 with the dimension "b" held constant at unity for a 9-line approximation. Only the average orders of magnitude of the final result at $x = a$ are included to show the degree to which the imposed boundary conditions were satisfied.

TABLE 4.7

DIRICHLET BOUNDARY-VALUE PROBLEM RESULTS
FOR A 9-LINE APPROXIMATION OVER A UNIT SQUARE

TIME STEP Δt	MIDPOINT SOLUTION Computed	Analytic	AVERAGE ERROR AT $x = 1$*	AVERAGE ERROR AT $x = 0.5$**
1	.04841	.04841	1.E-12	1.E-14
1/4	.16907	.16907	1.E-11	1.E-14
1/16	.44870	.44870	1.E-10	1.E-13
1/64	.76502	.76502	1.E-10	1.E-13
1/256	.92869	.92869	1.E-08	1.E-13
1/1024	.98116	.98116	1.E-03	1.E-09
1/4096	.99520	.99522	1.E+08	1.E-03

* Average order of magnitude of solution over all lines.

** Average order of magnitude of derivative over all lines.

TABLE 4.8

DIRICHLET BOUNDARY-VALUE PROBLEM RESULTS
FOR A 9-LINE APPROXIMATION AND 0.001 TIME STEP

INTEGRATION INTERVAL a	AVERAGE ERROR AT $x = a$*
0.6	1.E-09
0.7	1.E-07
0.8	1.E-06
0.9	1.E-03
1.0	1.E-02
1.1	1.E-01
1.2	1.E+01
1.3	1.E+02
1.4	1.E+04
1.5	1.E+05

* Average order of magnitude of solution over all lines.

Application to an irregular boundary

To demonstrate the application of the method presented to a problem involving an irregular boundary and to determine whether the irregular boundary would adversely influence the stability of the numerical solution, the following problem was considered. The rectangular domain of the preceding Dirichlet problem was distorted into an irregular shape by reducing the length of the boundary line y = 0 by 0.5 units from the length of the boundary line y = b = 1 as shown in Figure 4.1.

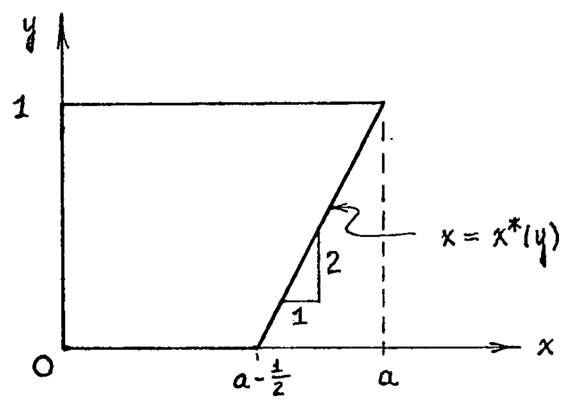

Figure 4.1 Irregular region in the xy-plane

The Dirichlet boundary conditions that the solution vanish over the entire boundary of the irregular region were retained from the preceding example and the initial distribution (3.3) was revised accordingly to

$$\theta(x,y,0) = \sin\frac{\pi x}{x^*} \sin \pi y \tag{4.7}$$

over the irregular region where

$$x^* = x^*(y) = a - \frac{1}{2} + \frac{y}{2} \tag{4.8}$$

is the equation of the skew boundary resulting from the distortion. The method of lines formulation of the problem resulted in the multi-point boundary-value problem

$$\left.\begin{aligned} &D^2\varphi_i^K(x) + \varepsilon^2\varphi_i^K(x) = \mathcal{D}\varphi_i^K(x) \\ &\varphi_i^K(0) = 0 \\ &\varphi_i^K(x_i^*) = 0 \end{aligned}\right\} \quad i = 1, 2, \ldots, N \tag{4.9}$$

where the x_i^* denote points at which the N interior lines $y = y_i$ intersect the skew boundary. Table 4.9 indicates the results obtained for a 9-line approximation and various time increments for the case $a = 1$ using the fourth-order Runge-Kutta integration scheme with linear interpolation employed for defining the forcing term in the governing equations. The tabulated values are the final solution along the skew boundary and are presented to reflect the degree to which the zero boundary conditions were satisfied along the skew boundary at each of the nine lines. Table 4.10 presents similar results for the specific time increment 0.0001 for an experiment in which the parameter "a" was varied over the range $0.6 \leq a \leq 1.5$. The integration step

TABLE 4.9

IRREGULAR REGION BOUNDARY-VALUE PROBLEM RESULTS
FOR A 9-LINE APPROXIMATION WITH $a = 1$

TIME STEP Δt	COMPUTED SOLUTION AT SKEW BOUNDARY — Line number 1	2	3	4	5	6	7	8	9
.04	-1.E-14	5.E-14	-8.E-15	-5.E-13	2.E-12	-2.E-12	-5.E-12	2.E-11	-4.E-11
.03	4.E-14	-2.E-13	5.E-13	-5.E-13	-2.E-12	8.E-12	-2.E-11	2.E-11	-7.E-12
.02	-2.E-14	7.E-14	-4.E-13	2.E-12	-6.E-12	1.E-11	-2.E-11	5.E-12	2.E-11
.01	2.E-13	-1.E-12	5.E-12	-2.E-11	3.E-11	-4.E-11	3.E-11	1.E-11	-7.E-11
.008	4.E-14	-5.E-13	3.E-12	-1.E-11	5.E-11	-2.E-10	5.E-10	-1.E-09	2.E-09
.006	-6.E-13	3.E-12	-6.E-12	-3.E-12	8.E-11	-4.E-10	1.E-09	-3.E-09	4.E-09
.004	1.E-12	-7.E-12	3.E-11	-9.E-11	2.E-10	-4.E-10	1.E-09	-4.E-09	9.E-09
.002	7.E-12	-7.E-11	3.E-10	-2.E-09	9.E-09	-4.E-08	1.E-07	-4.E-07	9.E-07
.001	5.E-11	-3.E-09	1.E-08	9.E-08	-1.E-06	-7.E-07	2.E-05	-2.E-04	5.E-04

TABLE 4.10

IRREGULAR REGION BOUNDARY-VALUE PROBLEM RESULTS
FOR A 9-LINE APPROXIMATION WITH $\Delta t = 0.001$

INTERVAL LENGTH a	COMPUTED SOLUTION AT SKEW BOUNDARY								
	Line number								
	1	2	3	4	5	6	7	8	9
0.6	-1.E-17	-2.E-14	-5.E-14	-6.E-13	8.E-13	2.E-12	-2.E-11	1.E-11	-9.E-11
0.7	-8.E-16	-2.E-14	2.E-14	-3.E-12	2.E-11	-6.E-11	-2.E-10	-2.E-09	3.E-10
0.8	2.E-13	-2.E-12	5.E-12	-8.E-11	-9.E-11	2.E-09	-3.E-08	1.E-08	1.E-07
0.9	4.E-12	-5.E-11	7.E-10	-1.E-08	5.E-08	-1.E-07	3.E-08	6.E-07	-4.E-06
1.0	-4.E-10	3.E-09	-3.E-08	1.E-07	-4.E-07	-1.E-06	4.E-06	1.E-05	-1.E-04
1.1	-2.E-08	1.E-07	-7.E-07	4.E-06	-2.E-05	2.E-04	-1.E-03	5.E-03	-1.E-02
1.2	7.E-07	-7.E-06	4.E-05	-2.E-04	9.E-04	-6.E-05	-3.E-02	2.E-01	-6.E-01
1.3	9.E-06	-1.E-04	7.E-04	-3.E-03	2.E-02	-1.E-01	9.E-01	-5.E 00	2.E+01
1.4	2.E-04	-1.E-03	7.E-03	-3.E-02	-2.E-01	4.E 00	-3.E+01	1.E+02	-2.E+02
1.5	8.E-03	-9.E-02	8.E-01	-6.E 00	2.E+01	-3.E 00	-7.E+02	5.E+03	-2.E+04

in both cases was chosen as 0.05, a convenient value which allowed the integration to step directly to each of the points x_i^* at which the boundary conditions were imposed. As can be seen from the results presented in Tables 4.9 and 4.10, the irregular boundary did not produce any apparent adverse effect on the stability of the numerical solution.

Discussion

The example problems presented in the preceding sections of this chapter illustrate the generality of the approach presented in this paper. A single general purpose computer program for the solution of linear multi-point boundary-value problems governed by systems of first-order ordinary differential equations was used in the solution of all boundary-value problems associated with these examples. The only modifications which were necessary involved the addition of a capability for repetitive solution of the resulting sequence of boundary-value problems at successive stages in time. Various boundary conditions along the regular regions were handled routinely with this approach and the irregular region of the last example presented no additional programming difficulty.

Attention was focused primarily on determining the ability of the method of particular solutions to obtain meaningful solutions at the first time stage rather than obtaining solutions over extended time stages. The closed-form solutions obtained for the example problems over the rectangular regions indicate the behavior of the numerical solution over extended time stages provided that a meaningful solution can be obtained for the first time stage. The time history of the numerical solution at four points corresponding to the midpoints of the even-numbered lines of a 9-line approximation over the irregular region is shown in Figure 4.2 for the case $a = 1$ and $\Delta t = 0.05$. The results were obtained using Runge-Kutta integration with step size $h = 0.05$. The analytic solution is not known; however, the results appear reasonable.

The unstable character of the system of ordinary differential equations arising from the method of lines reduction presented difficulties as expected in obtaining numerical solutions for small time increments. However, the unknown initial values of the desired solution were identified to high accuracy even in cases where the final result showed definite numerical instability. Imposing stricter convergence criteria did not alter the instability nor affect these initial values. Consequently, it was concluded that the IBM 360/44 word length was not of sufficient size to permit meaningful solutions for the smaller time increments. A comparison run was made on a CDC 6600 computer capable of carrying approximately twenty-nine significant figures in double

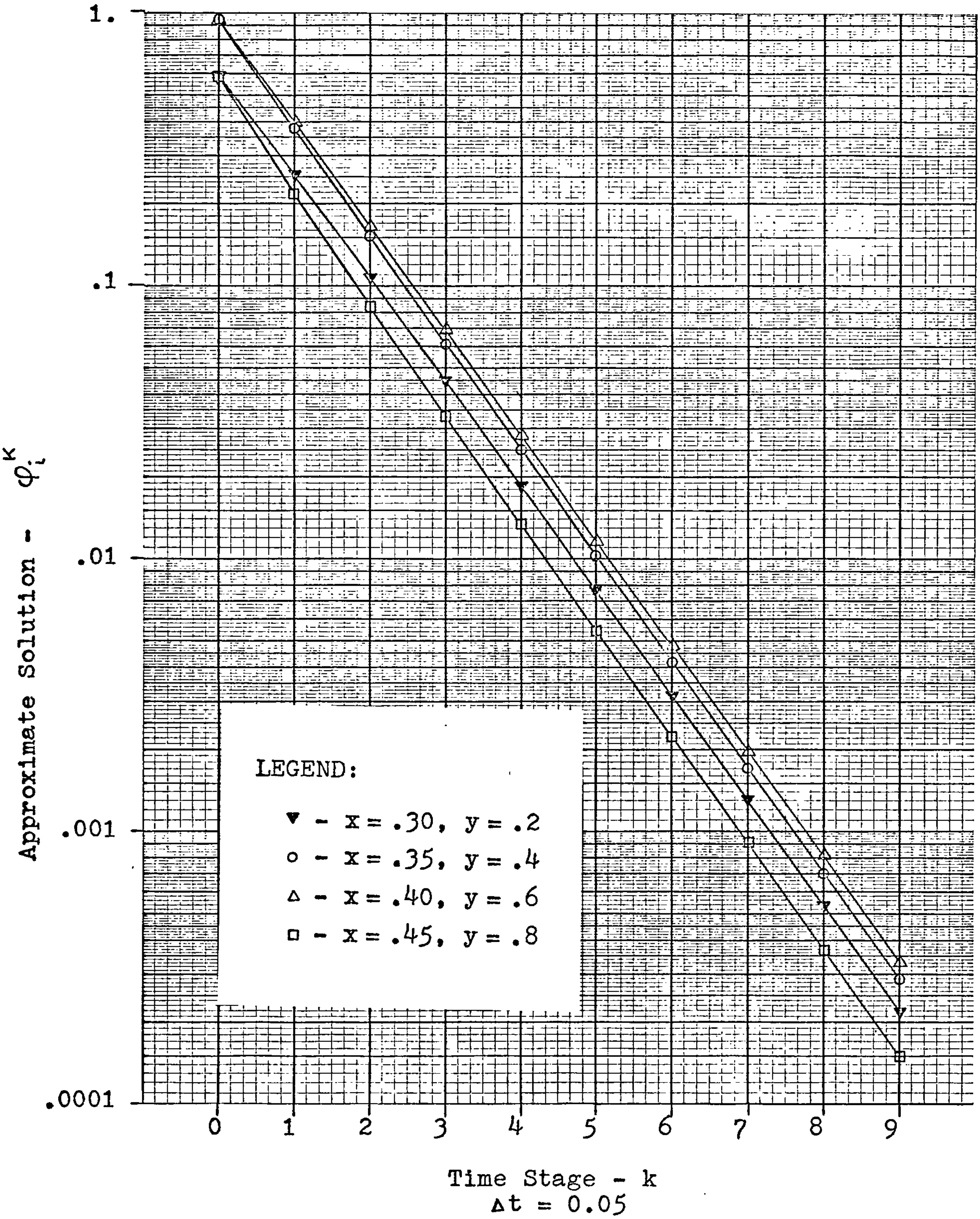

Figure 4.2 Time history of numerical solution at four selected points in the interior of the irregular region

TABLE 4.11

CDC 6600 COMPARISON RUN
MIXED BOUNDARY-VALUE PROBLEM RESULTS
FOR A 9-LINE APPROXIMATION WITH REVERSE INTEGRATION

TIME STEP Δt	COMPUTED SOLUTION FOR $y = 0.5$ $x = 0$	$x = 1$	AVERAGE ERROR AT $x = 0$*
1	.14110	.04428	1.E-21
1/4	.45917	.12102	1.E-21
1/16	1.06913	.17172	1.E-21
1/64	1.63236	.10232	1.E-20
1/256	1.89186	.03449	1.E-19
1/1024	1.97170	.00937	1.E-14

* Average order of magnitude of derivative over all lines.

precision arithmetic. The problem chosen for this test run was the mixed problem with the integration performed in the reverse direction, i.e., from $x = 1$ to $x = 0$. The results of this run are shown in Table 4.11 and may be compared with the results shown in Table 4.5. The significant increases in accuracy and stability emphasize the necessity of retaining as much precision as possible in the calculations.

The approach taken in this presentation in an attempt to control the instability of the system of equations resulting from the method of lines reduction was to combine the method of particular solutions with a power series integration scheme capable of high accuracy. This technique proved effective but showed a tendency to yield inaccurate results for very small time steps. Conte [9] has applied an orthonormalization scheme coupled with standard superposition techniques employing a constant step Runge-Kutta method to obtain impressive results for equations with large eigenvalues using single precision arithmetic on an IBM 7094. However, it is not clear to the author whether or not the technique can be applied to the equations of this particular problem with the same reported success.

CHAPTER V

SUMMARY AND CONCLUSIONS

The method of lines has been employed to reduce the general boundary-value problem governed by the two-dimensional diffusion equation to a sequence of related boundary-value problems which are governed by an inhomogeneous system of ordinary differential equations at selected stages in time. The dependence of the inhomogeneous terms only on the solution of the boundary-value problem at the preceding time stage permitted the numerical solution of the boundary-value problems by the method of particular solutions at successive time stages. Numerical examples included a problem of Dirichlet type and a problem of mixed type over a rectangular region, indicating the generality of boundary conditions which can be handled with this approach. A third numerical example demonstrated the ease with which irregular boundaries can be handled.

The stability of the numerical solutions indicated a high degree of dependence on the separation of the time stages, the numerical integration scheme used, and the length of the integration interval. This behavior was shown to arise from the unstable nature of the equations being integrated by determining the character of the general solution of the system at each time stage. The eigenvalues of the system were shown to increase rapidly with decreasing time step, resulting in sufficient amplification of small errors in the computations to obliterate completely the desired solution for sufficiently small time steps or for sufficiently long integration intervals.

Closed form solutions were obtained for specific problems by means of a separation of variables technique. The solutions so obtained were used to demonstrate the theoretical convergence of the solution to that of the original problem and to serve as a standard for evaluating the accuracy of the numerical solutions. It was concluded that reasonable accuracy could not be expected without a small time step whereas the effect of the line spacing was not so pronounced. This, coupled with the stability problems, necessitated a highly accurate numerical integration scheme.

Of the integration schemes considered, the power series technique proved most effective. In addition to obtaining more reliable results than the constant step fourth-order Runge-Kutta scheme, the computational time and storage requirements were significantly reduced with the power series technique using only one point of expansion. Test runs showed that the instability associated with the power series technique could be traced directly to computer limitations in word length rather than exceeding the radius of convergence of the power series expansion about the start of the interval.

In conclusion, the apparent advantages of the method presented appear to lie in its ease of application to a broad class of problems of the type presented. The question of nonlinear forms of the diffusion-type equation has not been considered. The feasibility of using this approach, coupled with the technique of quasilinearization, on nonlinear problems would appear to be the logical choice as the subject of future research. The full potential of the method, however, will probably not be realized until significant advances have been achieved in the development of improved computing hardware and software.

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