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Inverse Problems
in Partial
Differential Equations

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and
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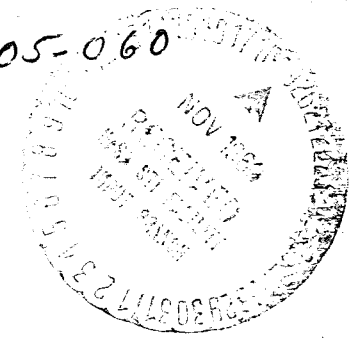
PROJECT THEMIS
Information Processing
Systems

INVERSE PROBLEMS IN PARTIAL

DIFFERENTIAL EQUATIONS

by

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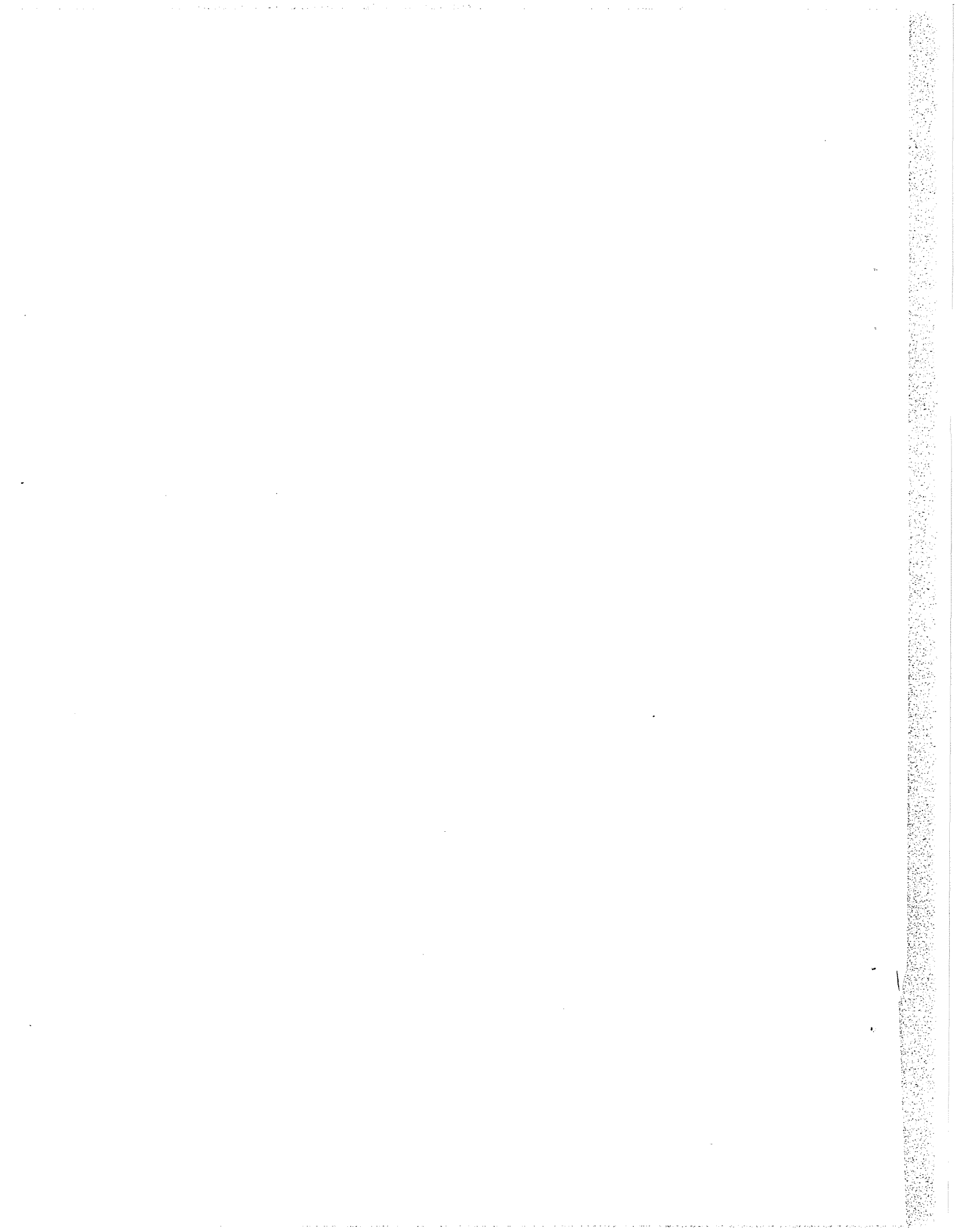

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FOREWORD

The University of Houston under a Department
of Defense, Project THEMIS grant, Office of Naval
Research Contract N00014-68-A-0151 is engaged in the
development of a computer information system in sup-
port of design, simulation and command/control. One
aspect of the project is the development of general
purpose computer programs for systems analysis. The
present report is the analytical phase of a system
identification (generalized mathematical modeling)
package based on quasilinearization. A user-oriented
computer software subsystem is available to aid in
the application of the process described in this re-
port and will be described in a subsequent user's
manual. Additional information on the availability
of the program and its relation to an integrated
design and simulation system may be obtained from:
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ABSTRACT

A procedure for identification in partial differential equations is described and illustrated by the Laplace equation and the unsteady heat conduction equation. The procedure for solution involves the substitution of difference operators for the partial derivatives with respect to all but one of the independent variables. The linear boundary value problem is solved by superposition of particular solutions. For nonlinear boundary value problems which arise from the original form of the equation or from the identification procedure, a Newton-Raphson-Kantorovich expansion in function space is used to reduce the solution to an iterative procedure of solving linear boundary value problems.

For the problems considered, this procedure has proven to be effective and results in a reasonable approximation to the solution of the boundary value problem in partial differential equations. For the identification problem, it is shown that the constant parameters are identified to the same accuracy as the supplementary data used in the identification procedure.

Incorporated in this identification procedure is the possibility in the case of overspecified data of meeting certain boundary conditions exactly and satisfying the remaining in a "best-fit manner."

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NOMENCLATURE

$\overline{\alpha}$	Vector of Unknown Initial Conditions
$\overline{\gamma}$	Vector of Superposition Constants
β	Perturbation Factor
S	Matrix Formed by Q_i Operator
Q_i	Operator which Indicates Time and State Variable of the ith Boundary Condition
J_o	Zeroth Bessel Function of the First Kind
γ	First Zero of J_o
ς	Arbitrarily Small Constant
Φ, Φ_p	Matrix of Independent Particular Solutions
$\overline{P}$	Solution Vector of Non-Homogeneous Equation
$\overline{V}$	Vector of State Variables
$\overline{u}$	Vector of Continuous Variables
$\overline{U}$	Vector of Approximate Variables
k	Iteration of the Linearized Equation
q	Sum of Unknown Constants and Unknown Initial Conditions
$\underline{d}$	Is Defined by
ℓ	Number of Boundary Values
E	Difference Operator
$\overline{C}$	Vector of Constant Coefficients

CHAPTER I

INTRODUCTION

Inverse problems in systems of differential equations have received considerable attention in the past few years. The applications of the techniques to solve these problems are being used in many areas of engineering and medical research.

In this dissertation we shall consider a type of inverse problem in which it is required to determine some of the coefficients in a partial differential equation. This type of inverse problem is also referred to as an identification problem.

In general, the present easily solved, numerically or analytically, identification problems are limited to ordinary differential equations. We will consider the application of one of these numerical techniques to partial differential equations and show that a large number of these can be solved with a reasonable labor.

This method uses quasilinearization. In the past few years many papers have been written showing how quasi-linearization may be used to solve boundary value problems of nonlinear ordinary differential equations. This same procedure used to solve the boundary value problem can be used for the identification of constant coefficients by

adding the differential equation for these constants and increasing the order of the system of equations.

Many of the problems of nonlinear partial differential equations are formidable in analytic form and researchers have relied on approximate techniques to solve these equations. This dissertation will be involved with the numerical integration of a set of ordinary differential equations resulting from an approximate method for solving partial differential equations.

One approximate method which has been studied in recent literature is known as the "method of lines" or "reduction to differential-difference equations" (see Appendix A)[1] The ordinary differential equations resulting from this approximation have been solved analytically in a few cases [1,2,3] and shown for general classes of linear problems to converge to the continuous solution as the discretizations are made arbitrarily small [4,5]. This approximation will be used to facilitate the solution of boundary value problems and the inverse problem associated with it.

The method of reducing partial differential equations to ordinary differential equations and the method of identification are discussed in Chapter II. A discussion

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[1]Appendix A is a definition of terms used in the dissertation

of boundary value problems will also be included in this chapter since the solution of such problems is an integral part of the method of identification.

The numerical results of the examples illustrated in Chapter II are given in Chapter III. Examples are shown of the identification of stable and unstable equations. Solutions of boundary value problems for both linear and nonlinear equations are illustrated with numerical considerations. A strategy for solving boundary value problems which become unbounded is also discussed in Chapter III. This strategy is an imbedding procedure and will be referred to as the method of similar boundary value problems. This will be illustrated for a mildly nonlinear equation.

Chapter IV contains the summary, conclusions, and recommendations for further work.

Statement of Problem

The problem is to describe and demonstrate the use of a method of solving the inverse problem which identifies parameters in partial differential equations. This method is based on quasilinearization [6] which has been successfully used for identification in both linear and nonlinear ordinary differential equations. This dissertation will show an identification procedure which can be applied to a

partial differential equation which has been reduced to a
set of ordinary differential difference equations.

Both stable and unstable equations will be investi-
gated to find what limitations are placed on such an
identification procedure when there is some doubt as to
their stability. Also, the problem of dimensionality will
be discussed with relationship to accuracy and computer
time. In addition, it is necessary to discuss the numerical
solution of the boundary value problem which results from
the method of reduction to ordinary differential equations.

Previous Work

The relative importance of techniques for solving
inverse problems has been recognized for several years.
Both statistical and deterministic methods of identifi-
cation have been developed for ordinary differential
equations. In the past few years some effort has been
made to extend these methods of identification to partial
differential equations.

Perdreauville [7] discusses the extension of the
method of Shinbrot [8]. This method does not obtain a
solution of the partial differential equation but results
in the evaluation of integrals over the domain which are
evaluated by use of the physical data. This method is
applicable only to equations whose elements can be

integrated by parts. However, he has illustrated that some alterations can be made to certain equations which are not directly integrable by parts.

Jones and Douglas [9] have shown the existence and uniqueness of the determination of a coefficient in the one dimensional unsteady heat conduction problem. Cannon [10] considers the existence and uniqueness of another type of inverse problem which is the determination of an unknown heat source from overspecified data.

One of the deterministic methods which has been developed is the use of quasilinearization to solve a nonlinear system of ordinary boundary value problems. The method is easily adapted to an identification procedure by coupling the differential equations for constants to the system and solving the boundary value problem. The development of these procedures was initiated by Bellman and Kalaba [6]. Holloway [11] used these ideas to investigate the feasibility of identification of the earth's geopotential from data of a synchronous satellite. Paine [12] reviews the use of quasilinearization in the computation of optimal control. The solution of nonlinear ordinary differential equations with non-linear boundary values was considered by Lee [13].

To directly use the ideas already developed for ordinary differential equations, it is necessary to reduce

the partial differential equation to a system of ordinary equations. Detchmendy [14] used the transformation of the independent variables as one method of reduction and characteristics in hyperbolic equations as a second method of reduction. The method of transformation requires the transformation of boundary conditions and the inverse transform to obtain the solution in its original coordinates. The method of characteristics is applicable to only a special type of partial differential equation.

The method of reduction employed in this dissertation is called the "method of lines" [1,4] or "analog solution" [15,16]. It is an approximate method which has been investigated primarily because it reduces the partial differential equation to a system of ordinary equations. The convergence of the approximate solution to the continuous solution has been considered by several authors. Lebedev [4] illustrates the application for a number of problems and establishes the convergence of the solution for some of these equations. Establishment of convergence and estimates of the error of the approximate solution have been considered in a number of papers [5,15,17,18] for particular linear heat conduction equations.

This approximate method is also referred to as the analog solution because of its applicability to analog computers. The approximate solution of a limited number of

linear parabolic and hyperbolic equations are considered in references [16,19-23]. Fisher [16] discusses the use of higher order approximations of derivatives for obtaining a more accurate solution. Greenwood [21] makes a comparison of a higher order scheme with lower order schemes for the beam vibration problem and shows that the increase of accuracy is significant.

This method is referred to in Russian literature as the "method of lines." Lebedev [4] states that "from a methodological point of view it should be more correctly called the differential-difference method or the differential-difference Fourier method." In all the examples which Lebedev considered, separation of variables was possible which led to Fourier series and thus the connection with the Fourier method is obvious. Two of the recently translated papers [1,2] have shown the explicit solution of these equations by reducing them to a canonical form and solving the resulting equations in the transformed space.

One of the more complete analytical references on the method of lines is a text by Berezin and Zhidkov [3] which also includes a number of references to earlier Russian literature.

Boyd [24] has used this approximate method for a solution of the Hemholtz equation in a spherical coordinate

system.

Sarmin and Chudov [25] have presented the analysis of stability of the integration of the resulting ordinary differential equations by a fourth order Runge-Kutta method and various orders of Adams methods. The models used in this analysis were

$$\frac{\partial u}{\partial x} = c \ \frac{\partial u}{\partial y}$$

$$\frac{\partial u}{\partial x} = c \ \frac{\partial^2 u}{\partial y^2}$$

and tables of limits were given for stability with respect to Cauchy data.

CHAPTER II

THEORY OF SOLUTION

Reduction to a Set of Ordinary Differential Equations

The reduction of a partial differential equation to a set of ordinary differential equations by the use of difference operators leads to an approximate method of solving partial differential equations. Since the solution is found along continuous lines, this method is referred to in Russian literature as the "method of lines." In other papers it is often referred to as the analog solution since this form of approximation is well suited to the use of analog computers.

The approximation is attained by substituting difference operators for the partial derivatives with respect to all but one of the independent variables. Thus, the equation depends only on one independent variable and is reduced to a set of ordinary differential-difference equations.

For illustration purposes, consider the following second-order partial differential equation

$$u_{xx} = g(u, u_y, u_{yy}, x, y) \qquad (2.1)$$

By assuming that u(x,y) is sufficiently smooth, we may

replace the derivatives with respect to the y direction by the finite difference approximations

$$\frac{\partial u}{\partial y}\bigg|_{y=y_i} \approx E^1(u(x,y_i))$$

$$\frac{\partial^2 u}{\partial y^2}\bigg|_{y=y_i} \approx E^2(u(x,y_i))$$

Thus Eq. (2.1) reduces to a system of ordinary differential equations

$$\frac{d^2 U_i}{dx^2} = g(U_i, E^1(U_i), E^2(U_i), x, y_0 + ih) \qquad (2.2)$$
$$1 \leq i \leq n$$

where

$$U_i \stackrel{d}{=} U_i(x) \approx u(x, y_0 + ih)$$

The choice of E^1 and E^2, which are finite difference operators, is important to the nature of the solution. Throughout this dissertation the order of an operator will have reference to the order with respect to its error.

The first and most basic approach is to use second order central difference approximations for the derivatives. The convergence proofs given by Douglas [18], Landau [15], and Friedman [17] were based on such a second order approximation in the unsteady heat conduction equation. Associated with such an approximation is an

error which will be termed the truncation error. This truncation error may be made arbitrarily small, but the required number of equations to be solved can become cumbersome.

Another alternative suggested by Fisher [16] is the use of higher order difference operators for the derivatives. This alternative does not complicate the method of solution, but instead leads to greater accuracy than is characteristic of the lower order approximation. Fisher shows that if the same higher order operator is used for all lines, additional boundary values are required and "spurious roots" are introduced into the solution. For example, consider E^2 to be a fourth order central difference operator which requires values for U_{i+2}, U_{i+1}, U_i, U_{i-1} and U_{i-2}. For lines $i = 1$ and $i = n-1$ values would be required for U_{-1} and U_{n+2} where U_0 and U_{n+1} are known boundary values. Fisher suggests that where the boundary values $U_0(x)$ and $U_{n+1}(x)$ are known explicity that U_{-1} and U_{n-1} be calculated by imposing the differential equation itself together with the second order approximations,

$$U_i = (U_{i-1} - U_{i+1})/2$$

$$E(U_i) = (-U_{i-1} + U_{i+1})/2 \Delta y \qquad (2.3)$$

$$E^2(U_i) = (U_{i-1} - 2U_i + U_{i+1})/\Delta y^2$$

For Eq. (2.1) the imposed condition is

$$\frac{d^2 U_o}{dx^2} = g(U_{-1}, U_o, U_1, x, y_o)$$ (2.4)

where $d^2 U_o/dx^2$ is known and Eqs. (2.3) have been substituted into Eq. (2.2). U_{-1} is the only unknown in Eq. (2.4) and its value is used to complete the fourth order approximation. In like manner, U_{n+1} may be found.

The extra boundary conditions and "spurious roots" may be avoided by using a difference approximation of the same higher order which includes only interior lines and the boundary. This requires special formulas for outer lines, but it does avoid the necessity of introducing extra boundary conditions.

As an illustration, consider a simulation of the Laplace equation

$$\frac{d^2 U_i}{dx^2} = - E^2(U_i) \qquad 1 \le i \le n$$ (2.5)

where

$$E^2(U_i) = (U_{i+2} + 16 U_{i+1} - 30 U_i + 16 U_{i-1} - U_{i-2})/12 \Delta y^2$$ (2.6)

$$1 \le i \le n$$

Writing Eq. (2.6) at $i = 2$ requires us to solve for U_1, U_o, and U_{-1}. Likewise, at $i = n$, U_n, U_{n+1}, and U_{n+2} are needed. This introduces the need for extra boundary conditions which may be found by imposing the differential equation.

Alternatively, these extra boundary conditions may be avoided by using the following fourth order approximations for the equations at i = 1 and i = n

$$E^2(U_1) = (U_5 - 6U_4 + 14U_3 - 4U_2 - 15U_1 + 10U_0)/12\,\Delta y^2$$

$$(2.7)$$

$$E^2(U_n) = (U_{n-4} - 6U_{n-3} + 14U_{n-2} - 4U_{n-1} - 15U_n + 10U_{n+1})/12\,\Delta y^2$$

$E^2(U_i)$ is known for all lines and is dependent only on the given boundary conditions and lines interior to the domain.

Presented in Chapter III are results which show that this higher order approximation gives better accuracy for a reasonable number of lines without additional expense in calculation. At this stage, the term reasonable number of lines is nebulus. However, it will become more clear as the method is described and the numerical results are presented.

Lebedev [4] has considered another line method of approximation which is of fourth order accuracy. The second order central difference approximation is expanded by a Taylor series about $u(x, y_i)$

$$u(x, y_{i+1}) - 2u(x, y_i) + u(x, y_{i-1})$$

$$= u(x, y_i + h) - 2u(x, y_i) + u(x, y_i - h)$$

$$= u(x, y_i) + h\frac{\partial u}{\partial y}\bigg|_{y_i} + \frac{h^2}{2!}\frac{\partial^2 u}{\partial y^2}\bigg|_{y_i} + \frac{h^3}{3!}\frac{\partial^3 u}{\partial y^3}\bigg|_{y_i}$$

$$+ \frac{h^4}{4!} \frac{\partial^4 u}{\partial y^4}\bigg|_{y_i} - 2u(x,y_i) + u(x,y_i) - h\frac{\partial u}{\partial y}\bigg|_{y_i}$$

$$+ \frac{h^2}{2!} \frac{\partial^2 u}{\partial y^2}\bigg|_{y_i} - \frac{h^3}{3!} \frac{\partial^3 u}{\partial y^3}\bigg|_{y_i} + \frac{h^4}{4!} \frac{\partial^4 u}{\partial y^4}\bigg|_{y_i}$$

$$= h^2 \frac{\partial^2 u}{\partial y^2}\bigg|_{y_i} + \frac{h^4}{12} \frac{\partial^4 u}{\partial y^4}\bigg|_{y_i} + o(h^6) \qquad (2.8)$$

and likewise

$$\frac{\partial^2 u}{\partial y^2}\bigg|_{y_{i+1}} - 2\frac{\partial^2 u}{\partial y^2}\bigg|_{y_i} + \frac{\partial^2 u}{\partial y^2}\bigg|_{y_{i-1}} = h^2\frac{\partial^4 u}{\partial y^4}\bigg|_{y_i} + o(h^4) \qquad (2.9)$$

Thus, by eliminating $\partial^4 u/\partial y^4$

$$u(x,y_{i+1}) - 2u(x,y_i) + u(x, y_{i-1})$$

$$= \left(\frac{\partial^2 u}{\partial y^2}\bigg|_{y_{i+1}} + 10\frac{\partial^2 u}{\partial y^2}\bigg|_{y_i} + \frac{\partial^2 u}{\partial y^2}\bigg|_{y_{i-1}} \right) h^2/12 - o(h^4) \qquad (2.10)$$

If the original partial differential equation is solved for $\partial^2 u/\partial y^2$ and substituted into Eq. (2.10), the resulting equation will be an approximation of fourth order.

As an illustration, consider the Laplace equation

$$u_{xx} + u_{yy} = 0 \qquad (2.11)$$

Solving for u_{yy} in Eq. (2.11) and substituting into Eq. (2.10)

$$\frac{1}{12}\left(\frac{d^2 U_{i+1}}{dx^2} + \frac{d^2 U_i}{dx^2} + \frac{d^2 U_{i-1}}{dx^2}\right) + h^2(U_{i+1} - 2U_i + U_{i-1})$$

$$+ h^2(U_{i+1} - 2U_i + U_{i-1}) = 0$$

$$\text{(2.12)}$$

Formulating Eq. (2.12) as a matrix equation,

$$A\frac{d^2\bar{U}}{dx^2} - F\bar{U}/h^2 = \bar{B} \qquad \text{(2.13)}$$

where

$$A = \frac{1}{12}\begin{bmatrix} 10 & 1 & 0 & \cdot & \cdot & \cdot & 0 & 0 & 0 \\ 1 & 10 & 1 & \cdot & \cdot & \cdot & 0 & 0 & 0 \\ 0 & 1 & 10 & \cdot & \cdot & \cdot & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \cdot & \cdot & \cdot & 1 & 10 & 1 \\ 0 & 0 & 0 & \cdot & \cdot & \cdot & 0 & 1 & 10 \end{bmatrix}$$

$$F = \begin{bmatrix} 2 & -1 & 0 & \cdot & \cdot & \cdot & 0 & 0 & 0 \\ -1 & 2 & -1 & \cdot & \cdot & \cdot & 0 & 0 & 0 \\ 0 & -1 & 2 & \cdot & \cdot & \cdot & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \cdot & \cdot & \cdot & -1 & 2 & -1 \\ 0 & 0 & 0 & \cdot & \cdot & \cdot & 0 & -1 & 2 \end{bmatrix}$$

$$\bar{B} = \frac{1}{12}\begin{bmatrix} \dfrac{d^2 U_0}{dx^2} + 12 U_0 \\ 0 \\ \vdots \\ 0 \\ \dfrac{d^2 U_n}{dx^2} + 12 U_n \end{bmatrix}$$

To be able to use this higher order approximation within the context of the methods discussed in this paper, it is necessary to reduce Eq. (2.13) to a system of first order equations. This may be accomplished by first multiplying Eq. (2.13) by A^{-1}

$$\frac{d^2\overline{U}}{dx^2} - A^{-1} F \overline{U} / h^2 = -A^{-1}\overline{B} \qquad (2.14)$$

then reducing Eq. (2.14) to its state variable form

$$\frac{d\overline{V_1}}{dx} = \overline{V_2}$$

$$\frac{d\overline{V_2}}{dx} = A^{-1} F \overline{V_1} / h^2 - A^{-1}\overline{B}$$

The Method of Identification

The method used here for identification of parameters in partial differential equations is based on the Newton-Raphson-Kantorovich expansion in function space. (see Appendix C) Bellman and Kalaba [6] refer to this as quasilinearization. This method reduces the solution of boundary value problems for nonlinear equations to an iterative process of solving boundary value problems for linearized equations. This method has been illustrated in several recent publications [6,11,12,13].

The particular details used in this study are closely associated with those used by Holloway [11] in the identification of constants of an ordinary differential equation.

Let us assume the general form of the partial differential equation given by

$$G_i\left(\bar{u}, \frac{\partial \bar{u}}{\partial \bar{x}}, \frac{\partial^2 \bar{u}}{\partial x^2}, \cdots \frac{\partial^m \bar{u}}{\partial x^m}, \bar{x}, \bar{c}\right) = 0$$

$$1 \leq i \leq n \qquad (2.14)$$

where $\bar{u}$ is an s dimensional vector and $\bar{x}$ is an r dimensional space representing r independent variables. $\bar{c}$ is a vector representing p constants appearing in the equation. The partial derivatives are noted as follows

$$\frac{\partial^i \bar{u}}{\partial \bar{x}^i} = \begin{bmatrix} \dfrac{\partial^i u_1}{\partial x_1^i} & \dfrac{\partial^i u_1}{\partial x_2^i} & \cdots & \dfrac{\partial^i u_1}{\partial x_r^i} \\[2mm] \dfrac{\partial^i u_2}{\partial x_1^i} & \dfrac{\partial^i u_2}{\partial x_2^i} & \cdots & \dfrac{\partial^i u_2}{\partial x_r^i} \\[2mm] \cdot & \cdot & \cdots & \cdot \\[2mm] \dfrac{\partial^i u_s}{\partial x_1^i} & \dfrac{\partial^i u_s}{\partial x_2^i} & \cdots & \dfrac{\partial^i u_s}{\partial x_r^i} \end{bmatrix}$$

To solve this set of n equations, we reduce Eq. (2.14) to a system of ordinary differential equations. As indicated before, this is done by substituting finite difference operators for the partial derivative operators with respect to all independent variables except one. The remaining variable x_1 will be referred to as the continuous variable and denoted as x. As described previously, the choice of finite difference approximations is somewhat arbitrary, but central difference approximations are generally used if it

is possible to do so without requiring extra boundary conditions to be imposed.

$$\frac{d^i \overline{U}}{dx^i} = \begin{bmatrix} \frac{d^i U_1}{dx^i} & E_2^i(U_1) & \cdot & \cdot & \cdot & E_r^i(U_1) \\ \frac{d^i U_2}{dx^i} & E_2^i(U_2) & \cdot & \cdot & \cdot & E_r^i(U_2) \\ \cdot & & \cdot & \cdot & \cdot & \cdot \\ \frac{d^i U_s}{dx^i} & E_2^i(U_s) & \cdot & \cdot & \cdot & E_r^i(U_s) \end{bmatrix}$$

The equations are reduced to the system of first order differential equations

$$\frac{d}{dx} \overline{V}_1 = \overline{f}(\overline{V}_1, \overline{h}, x, \overline{c}) \qquad (2.15)$$

where $\overline{f}$ is a vector function of $\overline{V}_1$, $\overline{h}$, x and $\overline{C}$. $\overline{V}_1$ is a vector of the state variables, $\overline{h}$ is the vector of increments of the independent variables which are discretized, and $\overline{C}$ is the vector of unknown constants.

The identification method can be described as follows:

(1) Adjoin to Eq. (2.15) the set of equations

$$\frac{d}{dx} \overline{C} = 0$$

which is the set of differential equations governing the unknown constants. Combine $\overline{V}_1$ and $\overline{C}$ into one vector

$$\overline{V} = \begin{bmatrix} \overline{V}_1 \\ \hline \overline{C} \end{bmatrix}$$

(2) Linearize Eq. (2.15) by the Newton-Raphson-Kantorovich expansion

$$\frac{d}{dx}\overline{V}^{k+1} = \overline{f}^{\,k} + \frac{\partial \overline{f}}{\partial \overline{V}}\bigg|^{k} (\overline{V}^{k+1} - \overline{V}^{k}) + H.O.T.$$

(2.16)

where k indicates the kth iteration

To solve Eq. (2.16) a solution k = 0 is required. Several methods have been proposed for obtaining this solution. One method is to estimate the values of the state variables and store these as $\overline{V}^{0}(x)$. A second method involves the integration of the nonlinear equations to obtain $\overline{V}^{0}(x)$. Thus, by assuming a vector of inital conditions $\overline{V}^{0}(o)$ and integrating the nonlinear Eqs. (2.15), $\overline{V}^{0}(x)$ is formed. $\overline{V}^{1}(x)$ can also be integrated using $\overline{V}^{0}(x)$ in Eq. (2.16).

The process of solving the linear boundary value problem is accomplished by the superposition of particular solutions. This simplifies the computer programming but increases the order of the matrix to be inverted in determining the proper initial conditions by one. In addition, the use of particular solutions has the feature of giving an explicit indication of the degree of convergence of the iterative process. (see Appendix B)

This method involves the perturbation of the initial conditions to insure that the resulting solutions will be independent and well behaved. In addition, this

perturbation process gives an explicit indication of the sensitivity of the solution to the initial conditions of the problem. This sensitivity is an important factor in the system identification process, especially in partial differential equations.

At this point, some indication should be given as to the order of the system of ordinary equations which will be solved. If Eq. (2.14) has r independent variables, $(r-1)$ of these are divided into n increments, then there will be $(r-1)(n-1)$ dependent variables for the approximate system of equations. When the approximate system is converted to a set of first order equations, the resulting system is $(r-1)(n-1)(m)$ where m is the highest order derivative with respect to the continuous independent variable. In addition, this set must be integrated $q+1$ times, where q is the number of the unknown initial conditions and unknown constants. Thus $(r-1)(n-1)(m)(q+1)$ equations must be integrated for each iteration. The order of the matrix to be inverted in solving for the new initial conditions is $(q+1)$.

It is not difficult to see that problems of dimensionality might be introduced if the increments of the discretized independent variables become too small, the number of independent variables become too large or the order of the derivative becomes too high. Although there

might be some difficulty due to dimensionality, the conceptuality of such a procedure is not destroyed and no limitations have been placed on the type of equations which can be handled by this method, except that the resulting ordinary differential equations should be quasilinear.

To illustrate the method, let us consider the Laplace equation within the domain of the unit square.

$$u_{xx} + c\, u_{yy} = 0 \qquad (2.17)$$

with classical boundary conditions,

$$u(1,y) = u(x,0) = u(x,1) = 0$$

$$u(0,y) = \sin \pi y \qquad (2.18)$$

To identify the parameter c, additional boundary values are required. Eq. (2.17) is expanded into its "lines form" which is

$$\frac{d^2 U_i}{dx^2} + c\, E^2(U_i) = 0 \qquad 1 \le i \le n$$

where n is the number of lines. Appendix D gives the analytical solution of a three line approximation for c = 1.

Let

$$V_i = U_i$$

$$V_{i+n} = dV_i/dx \qquad 1 \le i \le n$$

$$V_{2n+1} = c$$

Thus, the state variable vector is

$$\overline{V} = \left[\begin{array}{c} \overline{U} \\ \hline \dfrac{d\overline{U}\,/\,d\overline{x}}{C} \end{array} \right]$$

and the matrix equation is

$$\frac{d\overline{V}}{dx} = \overline{f}\,(\overline{V}, X, h)$$

The nonlinear equations are

$$\frac{dV_i}{dx} = V_{i+n} \qquad\qquad (2\text{-}19a)$$

$$\frac{dV_{i+n}}{dx} = -V_{2n+1}\ E^2(V_i) \qquad\qquad (2\text{-}19b)$$

$$\frac{dV_{2n+1}}{dx} = 0 \qquad\qquad (2\text{-}19c)$$

The linearized equations are formed by use of the linearization process already described. It is helpful to note that if E^2 is a linear operator on the state variables, it may be treated as a separate variable in the linearization procedure. Eq. (2.19a) and Eq. (2.19c) are already linear so that only Eq. (2.19b) needs to be expanded into a linear equation.

$$\frac{dV_{i+n}^{k+1}}{dx} = -V_{2n+1}^{k}\ E^2(V_i)^k + \left(V_{2n+1}^{k+1} - V_{2n+1}^{k}\right)\left(-E^2(V_i)^k\right)$$

$$+ \left(E^2(V_i)^{k+1} - E^2(V_i)^k\right)\left(-V_{2n+1}^{k}\right)$$

The resulting linearized equations are

$$\frac{dV_i^{k+1}}{dx} = V_{i+n}^{k+1}$$

$$\frac{dV_{i+n}^{k+1}}{dx} = -V_{2n+1}^{k} \; E^2(V_i)^{k+1} - (V_{2n+1}^{k+1} - V_{2n+1}^{k})E^2(V_i)^{k}$$

$$\frac{dV_{2n+1}}{dx} = 0 \tag{2.20}$$

Let us assume a three line approximation to the problem as shown in Fig. 2.1 and choose a second order central difference operator for E^2.

$$E^2(V_i) = (V_{i+1} - 2V_i + V_{i-1}) / h^2$$

The matrix equation is

$$\frac{d\bar{V}}{dx} = \left[\begin{array}{c|c} A_{11} & A_{12} \\ \hline A_{21} & A_{22} \end{array} \right] \bar{V} + \bar{B}$$

where

$$A_{12} = \begin{bmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -2 \\ 0 & 0 & 0 \end{bmatrix} \qquad A_{11} = [0]$$

$$A_{22} = \frac{1}{h^2}\begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \qquad A_{22} = [0]$$

V_1 and V_2 denote the boundary conditions at $y = 0$ and $y = 1$, respectively.
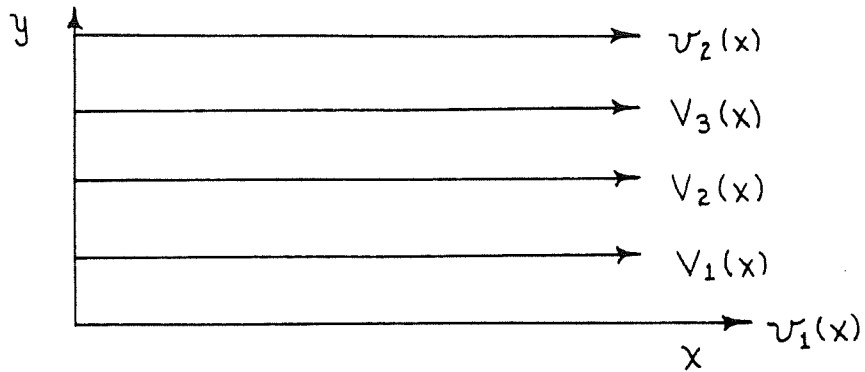
Figure 2.1 Three Line Approximation

The linearized equation may also be written in matrix form

$$\frac{d\overline{V}}{dx}^{k+1} = \left[\begin{array}{c|c} A_{11} & A_{12} \\ \hline A_{21} & A_{22} \end{array} \right]^{K} V^{k+1} - \overline{B}^{K}$$

where

$$A_{12} = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \qquad A_{11} = \begin{bmatrix} 0 \end{bmatrix}$$

$$A_{22} = \frac{1}{h^2} \begin{bmatrix} 0 & 0 & 0 & \upsilon_1 - 2V_1 + V_2 \\ 0 & 0 & 0 & V_1 - 2V_2 + V_3 \\ 0 & 0 & 0 & V_2 - 2V_3 + \upsilon_2 \\ 0 & 0 & 0 & 0 \end{bmatrix}^{K}$$

$$A_{21} = \frac{V_7^{k}}{h^2} \begin{bmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -2 \\ 0 & 0 & 0 \end{bmatrix}$$

For an initial approximation, k = 0, an initial vector $\overline{V}^0(o)$ is assumed which contains the known initial conditions and an estimate of the missing initial conditions from apriori knowledge. For the problem under consideration we choose

$$\overline{V}^0(o) = \begin{bmatrix} V_1(o) \\ V_2(o) \\ V_3(o) \\ \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \end{bmatrix} = \begin{bmatrix} u(o,h) \\ u(o,2h) \\ u(o,3h) \\ \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \end{bmatrix} \qquad (2.21)$$

where α_i, $1 \leq i \leq 4$, are the estimates of the missing initial conditions.

To find the solution of the linear boundary value problem shown in Eqs. (2.20), it is necessary to know $\overline{V}^0(x)$, which is obtained by solving the nonlinear Eqs. (2.19) with initial conditions Eq. (2.21). Eq. (2.20) is then integrated using the nonlinear solution and the initial vector Eq. (2.21). Since there are four unknown initial values, it is necessary to generate four independent solutions. We do this by perturbing the unknown initial conditions by some constant multiplier. We denote this constant as β which may be different for each unknown initial condition α_i. A fifth solution of the linearized equation is generated by using the unperturbed initial

conditions, Eq. (2.21).

Let $\Phi(x)$ be the solution matrix of the linearized
Eqs. (2.20) which obeys the equation

$$\frac{d\Phi}{dx} = A\Phi + D \qquad (2.22)$$

where $\qquad D = [\,\overline{B}\,|\,\overline{B}\,|\,\cdots\,|\,\overline{B}\,]$

and

$$\Phi(0) = \begin{bmatrix} V_1(0) & V_1(0) & V_1(0) & V_1(0) & V_1(0) \\ V_2(0) & V_2(0) & V_2(0) & V_2(0) & V_2(0) \\ V_3(0) & V_3(0) & V_3(0) & V_3(0) & V_3(0) \\ \beta\alpha_1 & \alpha_1 & \alpha_1 & \alpha_1 & \alpha_1 \\ \alpha_2 & \beta\alpha_2 & \alpha_2 & \alpha_2 & \alpha_2 \\ \alpha_3 & \alpha_3 & \beta\alpha_3 & \alpha_3 & \alpha_3 \\ \alpha_4 & \alpha_4 & \alpha_4 & \beta\alpha_4 & \alpha_4 \end{bmatrix}$$

Let Q_i represent the operator which indicates the
value of x and the state variable for which the boundary
condition, b_i, is known. With this operator notation, the
following linear equations must be solved for $\overline{\gamma}$.

$$b_i = \sum_{j=1}^{5} (Q_i \Phi(x_i))_j \gamma_j \qquad 1 \leq i \leq \ell \qquad (2.23)$$

The vector $Q_i \Phi(x_i)$ denotes the row of the matrix $\Phi(x_i)$
which corresponds to the state variable for which the ith
boundary condition is given.

Coupled with Eq. (2.23) is the auxilary condition
Eq. (2.24) required for the superposition of particular
solutions

$$\sum_{i=1}^{5} \gamma_i = 1 \tag{2.24}$$

Eqs. (2.23) and (2.24) may be combined in the following notation

$$\overline{b} = S \overline{\gamma} \tag{2.25}$$

where

$$S = \begin{bmatrix} Q_1 \Phi(x_1) \\ \hline Q_2 \Phi(x_2) \\ \vdots \\ \hline Q_\ell \Phi(x_\ell) \\ \hline 1 & 1 & \cdots & 1 \end{bmatrix}$$

As a second example, consider the unsteady heat conduction equation

$$\frac{\partial u}{\partial x} = c \frac{\partial^2 u}{\partial y^2} \tag{2.26}$$

with boundary conditions

$$u(x,0) = u(x,1) = 0$$
$$u(0,y) = \sin \pi y$$

The Cauchy problem is correctly posed for this equation, and it is expected that reasonable accuracy could be obtained in the identification of the parameter "c." This equation has been well studied, and its solutions are well known. As was indicated in Chapter I, the convergence of

the differential-difference equations is well established, and the stability of the numerical integration of the resulting equations was studied by Sarmin and Chudov [25]. For their studies, x was carried as the continuous variable.

The approximation of Eq. (2.26) results in the set of ordinary differential equations

$$\frac{dU_i}{dx} = c\ E^2(U_i) \qquad 1 \leq i \leq n \qquad (2.28)$$

with boundary conditions

$$U_o(x) = U_{n+1}(x) = 0$$

$$U_i(x) = \sin\ (i\pi/n+1)$$

The change of notation which has been used earlier in this chapter is helpful in conceiving Eq. (2.28) as a state variable type equation. Let $V_{n+1} = c$ so that the complete set of nonlinear equations to be solved is

$$\frac{dV_i}{dx} = V_{n+1}\ E^2(V_i)$$

$$\frac{dV_{n+1}}{dx} = 0 \qquad 1 \leq i \leq n$$

The linearized set of equations are

$$\frac{dV_i^{K+1}}{dx} = V_{n+1}^K\ E^2(V_i)^K + (V_{n+1}^{K+1} - V_{n+1}^K)\ E^2(V_i)^K$$

$$\frac{dV_{n+1}}{dx} = 0 \qquad 1 \leq i \leq n$$

The procedure for solution of these equations is the same as has been described for the Laplace equation.

Overdetermined System of Equations

If the number of known boundary conditions ℓ is greater than the number of unknown initial conditions, then S will not be a square matrix and Eq. (2.25) will not have a unique solution.

Among the most used methods of solving such problems of overdetermined systems is the method of least squares. A set of (q+1) equations may be formed by minimizing the square of the deviations from the given boundary conditions, $\overline{b}$

$$\min_{\overline{\gamma}} (\overline{b} - S\overline{\gamma})^T (\overline{b} - S\overline{\gamma})$$

where q is the number of unknown initial conditions. Carrying out this minimization with respect to the constants $\overline{\gamma}$ gives Eq. (2.29)

$$-S^T(\overline{b} - S\overline{\gamma}) - (b - S\gamma)^T S = 0$$
$$-2S^T(\overline{b} - S\overline{\gamma}) = 0$$

or
$$S^T\overline{b} = S^T S\overline{\gamma} \tag{2.29}$$

However, consider that ℓ boundary values are given such that $\ell \geq q$ where q is the number of unknown initial conditions and ℓ_1 of these are known exactly. The

remaining ℓ_2 are approximate boundary values to be fit in a least square sense. Let us partition Eq. (2.25)

$$\left[\begin{array}{c} \overline{b_1} \\ \hline \overline{b_2} \end{array}\right] = \left[\begin{array}{c|c} S_{11} & S_{12} \\ \hline S_{21} & S_{12} \end{array}\right] \left[\begin{array}{c} \overline{\gamma_1} \\ \hline \overline{\gamma_2} \end{array}\right]$$

so that we obtain two vector equations

$$\overline{b_1} = S_{11}\overline{\gamma_1} + S_{12}\overline{\gamma_2} \tag{2.30a}$$

$$\overline{b_2} = S_{21}\overline{\gamma_1} + S_{22}\overline{\gamma_2} \tag{2.30b}$$

Since $\overline{\gamma}_1$ is known from Eq. (2.30a), substitute it into Eq. (2.30b)

$$\overline{\gamma_1} = S_{11}^{-1}(\overline{b_1} - S_{12}\overline{\gamma_2})$$

$$\overline{b_2} = S_{21}S_{11}^{-1}(\overline{b_1} - S_{12}\overline{\gamma_2}) - S_{22}\overline{\gamma_2}$$

Minimizing the square of the deviations with respect to the remaining constants

$$\min_{\overline{\gamma_2}} \left(\overline{b_2} - S_{21}S_{11}^{-1}\overline{b_1} - (S_{22} - S_{21}S_{11}^{-1}S_{12})\overline{\gamma_2}\right)^T$$
$$\left(\overline{b_2} - S_{21}S_{11}^{-1}\overline{b_1} - (S_{22} - S_{21}S_{11}^{-1}S_{12})\overline{\gamma_2}\right)$$

giving

$$\left(\overline{b_2} - S_{21}S_{11}^{-1}\overline{b_1} - (S_{22} - S_{21}S_{11}^{-1}S_{12})\overline{\gamma_2}\right)^T$$
$$(S_{22} - S_{21}S_{11}^{-1}S_{12}) = 0 \tag{2.31}$$

Letting

$$S' = S_{22} - S_{21}S_{11}^{-1}S_{12}$$

$$(S')^T(\overline{b_2} - S_{21}S_{11}^{-1}\overline{b_1}) = (S')^T S'\overline{\gamma_2} \tag{2.32}$$

By substituting Eq. (2.30b) into Eq. (2.31)

$$(S')^T \bar{b}_2 = (S')^T (S_{21} \bar{\gamma}_1 + S_{22} \bar{\gamma}_2) \qquad (2.33)$$

$\bar{b}_1$ is the vector of ℓ_1 exact boundary conditions such that $0 \leq \ell_1 \leq q$. b_2 is the vector of ℓ_2 inexact boundary conditions such that $\ell_2 + \ell_1 > q$. $\bar{\gamma}_1$ contains the first ℓ_1 constants and ℓ_2 contains the remaining $(q - \ell_1)$ constants.

The auxiliary equation, Eq. (2.24) for the super-position of particular solutions is included in Eq. (2.30a).

If we consider the auxiliary equation to be the only exact equation, S_{12}^T is the unit vector, $\bar{S}_{12}^T$ is the unperturbed solution vector, and S_{11}^{-1} is a scalar and equal to 1. Thus

$$S' = S_{22} - \left[\bar{S}_{21} \mid \bar{S}_{21} \mid \cdots \mid \bar{S}_{21} \right]$$

or the columns of S are the difference between the perturbed solution vectors and the unperturbed vector. The boundary condition of Eq. (2.32) is altered in a similar manner

$$\bar{b}_2 - S_{21} S_{11}^{-1} \bar{b}_1 = \bar{b}_2 - \bar{S}_{21}$$

$$(S')^T (\bar{b}_2 - \bar{S}_{21}) = (S')^T S' \bar{\gamma}_2$$

Eq. (2.32) reduces to

$$(S')^T \bar{b}_2 = (S')^T (S_{21} \bar{\gamma}_1 + S_{22} \bar{\gamma}_2)$$

An approach which has proven to be successful in the problems we have considered is an alteration of the least square approach. This pseudo-least square method substitutes S_{22} in Eq. (2.33) for S'. Thus, in addition to Eq. (2.30a), the equation

$$S_{22} \, \overline{b}_2 = S_{22} \left(S_{21} \, \overline{\gamma}_1 - S_{22} \, \overline{\gamma}_2 \right) \qquad (2.34)$$

is used to solve for $\overline{\gamma}$.

Boundary Value Problems

In the example problems considered thus far, it has been assumed that the boundary conditions U_o and U_{n+1} are known. This requirement is convenient but not necessary. Consider the following problem

$$\Delta^2 u = J_o(2\gamma r) \qquad (2.35)$$

where Δ^2 is the Laplacian operator and γ is the first zero of J_o with the boundary conditions

$$\begin{array}{l} u(\theta, .5) = 0 \\ u(\theta, 0) = \text{finite} \\ u(\theta, r) = u(\theta + 2\pi, r) \end{array} \qquad (2.36)$$

The solution to this problem in cylindrical coordinates is

$$u(\theta, r) = - J_o(2\gamma r) / (2\gamma)^2$$

Let us consider this problem given on the domain of the unit square. The governing equation is

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = J_0(2\gamma r)$$

where $\quad r = ((.5 - x)^2 + (.5 - y)^2)^{.5}$

The approximate equations are

$$\frac{d^2 U_i}{dx^2} = -E^2(U_i) + J_0(2\gamma r) \quad 1 \le i \le n$$

with boundary conditions appearing at points interior to the boundary of the domain. Let n = 7 such that the square is divided into eight equal slabs as illustrated in Fig. 2.2.
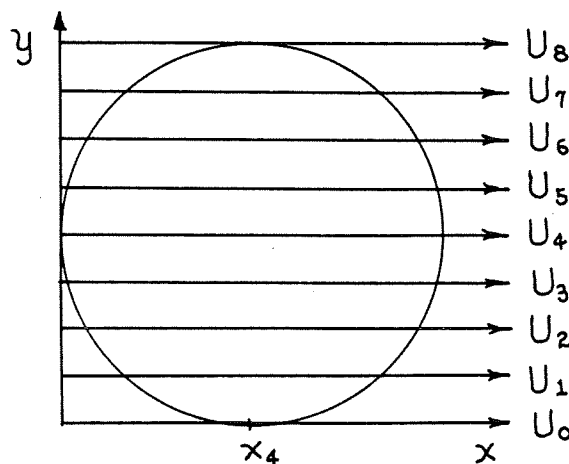
Figure 2.2 Line Approximation for
Circular Shaped Boundary

For this example, the functions $U_8(x)$ and $U_0(x)$ are not known. However, since $U_8(x_4)$ and $U_0(x_4)$ are known, we might consider making $U_8(x) = U_8(x_4)$ and $U_0(x) = U_0(x_4)$. However, this will lead to a poor approximation of $E^2(U_1)$.

For an alternate approach, we must realize that two additional boundary conditions can be found for $U_o(x)$ and $U_8(x)$.

$$\frac{d\,U_o(x)}{dx}\bigg|_{x=x_4} = 0$$

$$\frac{d\,U_8(x)}{dx}\bigg|_{x=x_4} = 0 \qquad (2.37)$$

Although we will refer to Eqs. (2.37) as boundary conditions for the approximate equation, they are not boundary conditions for the continuous problem. To show how these conditions arise, assume that $U_o(x)$ is a secant to the curve C as shown in Fig. 2.3.
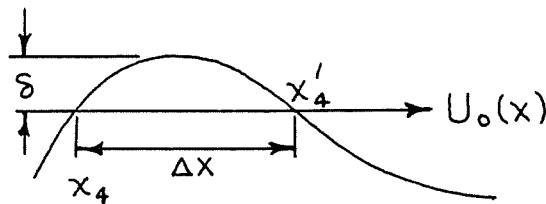
Figure 2.3 Tangent Boundary Condition

As δ is made arbitrarily small

$$\lim_{\delta \to 0} \frac{(U_o(x'_4) - U_o(x_4))}{\Delta x} = \frac{d\,U_o(x)}{dx}\bigg|_{x=x_4}$$

if the known function along the curve C is continuous.

A forward and backward finite difference approximation of second or fourth order is used for $E^2(U_o)$ and $E^2(U_8)$. This approach has proven to be successful for the problem being considered and the results will be discussed in Chapter III.

CHAPTER III

RESULTS AND CALCULATIONS

The results of the numerical calculations will
illustrate the accuracy of the solution to the boundary
value problems and the rate of convergence in identifi-
cation of constants in the partial differential equations.
The results are compared to analytical results in order to
obtain an estimate of the accuracy of the integration
procedure.

Laplace Equation

Identification in the Laplace equation was considered
since the Laplace equation is unstable when integrated as
an initial value problem, that is with Cauchy data. Fisher
[22] and Hartee [26] suggested that the elliptic equations
were unsuitable for solution on the analog computer because
of the instability of the approximate equations and the
difficulty of obtaining the correct initial conditions to
solve the boundary value problem.

In Chapter II, it was shown how the linear boundary
value problem can be easily solved so that there is little
difficulty in obtaining the correct initial conditions.
By the use of a finite domain and a greater number of
significant figures than is available on analog computers,

one is able to obtain a good approximation to the solution of the continuous problem and identify the parameters in the equation.

Tables 3.1 and 3.3 show the numerical solution of

$$\Delta^2 u = 0 \tag{3.1}$$

with boundary conditions

$$u(x,0) = u(x,1) = u(x_1,y)$$
$$u(0,y) = \sin \pi y \tag{3.2}$$

The analytical solution is

$$u(x,y) = \sin \pi y \left(\cosh \pi x - \frac{\cosh \pi x_1}{\sinh \pi x_1} \sinh \pi x \right) \tag{3.3}$$

The instability of this equation is exhibited by the fact that any error is propagated and grows as the basic solution of the equation grows.

The Laplace equation with Cauchy data is the classical example of an ill-posed problem of mathematical physics in the sense of Hadamard [27]. However, the consideration according to Tykhonov's formulation gives the possibility of constructing an approximate solution with a certain guaranteed degree of accuracy in spite of the fact that an exact solution of Eq. (3.1) with approximate Cauchy data does not exist at all or may strongly deviate from the true solution [28].

For the problem under consideration

$$\frac{\partial u}{\partial x} = -\pi \sin \pi y \frac{\cosh \pi x_1}{\sinh \pi x_1}$$

As x_1 is increased $\partial u / \partial x \big|_{x=0}$ approaches a limit. The
ill-posed nature is then illustrated by the fact that as
x_1 is increased and the same Dirchlet boundary conditions
are imposed, the change in the initial derivative of the
Cauchy data is decreased. Thus, a point is reached at
which changes of the initial derivative occur beyond the
number of significant figures carried by the computer, and
it would not be possible to find a slope which would meet
the boundary conditions with an error less than ϵ.

Both the instability and ill-posed nature must be
considered, but these problems do not eliminate the
possibility of identification for such equations. The
instability is inherent, but by an appropriate integration
scheme it is possible to keep integration errors smaller
than the truncation error which is due to the finite
approximation. The ill-posed nature is a constraint on the
method for the Laplace equation and means that associated
with x_1 is an error ϵ such that

$$\epsilon(x_1) = \max_{y_m} \big| u(x_1, y_m) - U_m(x_1) \big|$$

The solutions of the 3, 5 and 7 line approximation
with a second order central difference operator are shown

TABLE 3.1

APPROXIMATE SOLUTIONS OF THE LAPLACE EQUATION
USING 2ND ORDER DIFFERENCE OPERATORS

x	y	3 lines	5 lines	7 lines	Analytical
.1	.5	.7348	.7317	.7306	.7292
.25	.5	.4614	.4565	.4548	.4526
.5	.5	.2066	.2025	.2010	.1992
.75	.5	.0790	.0769	.0762	.0752
.9	.5	.0292	.0283	.0280	.0276
.1	.25	.5196	--	.5166	.5156
.25	.25	.3262	--	.3216	.3201
.5	.25	.1461	--	.1422	.1409
.75	.25	.0559	--	.0538	.0532
.9	.25	.0206	--	.0198	.0195
.1	.1667	--*	.3658	--	.3646
.25	.1667	--	.2282	--	.2263
.5	.1667	--	.1012	--	.0996
.75	.1667	--	.0384	--	.0376
.9	.1667	--	.0141	--	.0138

* no values are available

TABLE 3.2

DIFFERENCE BETWEEN ANALYTICAL AND APPROXIMATE
SOLUTIONS SHOWN IN TABLE 3.1

x	y	3 lines	5 lines	7 lines
.1	.5	-.0056	-.0025	-.0014
.25	.5	-.0088	-.0039	-.0022
.5	.5	-.0074	-.0033	-.0018
.75	.5	-.0038	-.0017	-.0010
.9	.5	-.0016	-.0007	-.0004
.1	.25	-.0040	--	-.0010
.25	.25	-.0061	--	-.0015
.5	.25	-.0052	--	-.0013
.75	.25	-.0027	--	-.0006
.9	.25	-.0011	--	-.0003
.1	.1667	--*	-.0012	--
.25	.1667	--	-.0019	--
.5	.1667	--	-.0016	--
.75	.1667	--	-.0008	--
.9	.1667	--	-.0003	--

* no values are available

in Table 3.1 and compared with the analytical solution.
The error in the approximate solutions from Table 3.1 is
shown in Table 3.2. Table 3.3 shows the increased accuracy
obtained by using fourth order operators for the deriva-
tives and in Table 3.4 the error in the solutions from
Table 3.3 is presented. This increase in accuracy is
significant and shows that for the chosen domain the
instability does not nullify the solution. The results in
Tables 3.1 and 3.3 were obtained with a predictor-corrector
integration program with a step size of .01. The maximum
number of corrections allowed was four.

A fourth order Runge-Kutta integration was used to
compare the results with that of the predictor-corrector.
The same step size was used and the run times were nearly
identical. However, as indicated in Table 3.5, the Runge-
Kutta was more accurate as x, the continuous variable,
increased. The time required to solve the linear boundary
value problem with seven lines was less than .5 minutes on
the Sigma VII digital computer.

The inverse problem was solved for

$$\frac{\partial^2 u}{\partial x^2} + c \frac{\partial^2 u}{\partial y^2} = 0 \tag{3.4}$$

with the same boundary conditions indicated in Eq. (3.2)
with values of u specified at points interior to the
domain.

TABLE 3.3

APPROXIMATE SOLUTIONS OF THE LAPLACE EQUATION
USING SEVEN LINES WITH 2ND AND 4TH
ORDER DIFFERENCE OPERATORS

x	y	2nd order	4th order	Analytical
.1	.125	.2795	.278995	.279056
.1	.375	.6750	.673690	.673700
.1	.5	.7306	.729202	.729208
.25	.125	.1740	.173167	.173236
.25	.375	.4202	.418206	.418229
.25	.5	.4548	.452677	.452688
.5	.125	.0769	.076215	.076257
.5	.375	.1857	.184076	.184100
.5	.5	.2010	.199247	.199268
.75	.125	.0291	.028767	.028785
.75	.375	.0703	.069479	.069492
.75	.5	.0761	.075205	.075218
.9	.125	.0107	.010576	.010582
.9	.375	.0259	.025542	.025548
.9	.5	.0280	.027648	.027652

TABLE 3.4

DIFFERENCE BETWEEN ANALYTICAL AND APPROXIMATE SOLUTIONS SHOWN IN TABLE 3.3

x	y	2nd order	4th order
.1	.125	.0005	.000061
.1	.375	.0013	.000010
.1	.5	.0014	.000006
.25	.125	.0008	.000069
.25	.375	.0020	.000023
.25	.5	.0022	.000011
.5	.125	.0007	.000042
.5	.375	.0016	.000024
.5	.5	.0018	.000021
.75	.125	.0004	.000018
.75	.375	.0007	.000013
.75	.5	.0009	.000013
.9	.125	.0002	.000006
.9	.375	.0004	.000006
.9	.5	.0004	.000004

TABLE 3.5

COMPARISON OF INTEGRATION PROCEDURES FOR THE
4TH ORDER, SEVEN LINE APPROXIMATION
OF THE LAPLACE EQUATION

x	y	Predictor-Corrector	Runge-Kutta	Analytical
.25	.125	.173167	.173179	.173236
.25	.375	.418206	.418233	.418228
.25	.5	.452677	.452699	.452688
.5	.125	.076215	.0762249	.076256
.5	.375	.184076	.184098	.184100
.5	.5	.199247	.199271	.199268
.75	.125	.028767	.028772	.028785
.75	.375	.069479	.069490	.069492
.75	.5	.075205	.075217	.075218

Table 3.6 shows the results of the calculations using three data points correct to four significant figures.

$$u(x_1,y_1) = u(.5,.125) = .0762$$
$$u(x_2,y_2) = u(.5,.25) = .1409$$
$$u(x_3,y_3) = u(.5,.5) = .1992$$

The initial estimate of the constant was chosen to deviate 10% from correct value and the initial derivatives were chosen as convenient values for input to the program which deviated by approximately 20%. The seven line approximation with predictor-corrector integration of step size .01 was used in the identification procedure. Seven iterations were required for this identification, and the constant, c, was identified to four significant figures as shown in Table 3.6 which is equivalent to the accuracy of the data.

Also shown in Table 3.6 are the initial conditions, α_i, at each iteration and the constants γ_i obtained from the matrix inversion. A perturb factor, β, of 1.0001 was necessary to keep the perturbed solutions of the same order of magnitude as the unperturbed solution. It may be observed that $(\beta - 1) \gamma_i$ is the percentage change in the initial conditions and that the constants γ_i, $1 \leq i \leq 7$, were adjusted so that they were approximately equal and converged uniformly and monotonically at a quadratic rate. Table 3.7 shows the accuracy to which the boundary values

TABLE 3.6

CONVERGENCE OF α_i, c and γ_i FROM IDENTIFICATION
IN THE LAPLACE EQUATION USING COMBINATION OF
EXACT AND INEXACT BOUNDARY CONDITIONS

Iteration	α_1/γ_1	α_2/γ_2	α_3/γ_3	α_4/γ_4	c/γ_8
0	-1.000000 1484	-2.000000 595	-3.000000 -782	-4.000000 -2530.	.9000000 -61.
1	-1.147197 1405	-2.118120 1406	-2.767302 1405	-2.995929 1399	.8998604 2898.
2	-1.307093 -195.	-2.413500 -196.	-3.153191 -196.	-3.411633 -193.	1.158533 -262.
3	-1.281690 -317.	-2.366484 -317.	-3.091725 -317.	-3.346128 -317.	1.128341 -640.
4	-1.241356 -204.	-2.291995 -204.	-2.994391 -204.	-3.240907 -204.	1.056709 -408.
5	-1.216146 -63.	-2.245425 -63.	-2.933515 -63.	-3.175112 -63.	1.013904 -125.
6	-1.208511 -5.	-2.231317 -5.	-2.915064 -5.	-3.155183 -5.	1.001303 -11.
7	-1.207805 -5. E-02	-2.230011 -5. E-02	-2.913356 -5. E-02	-3.153339 -5. E-02	1.000145 -.1
8	-1.207799 -1. E-05	-2.229999 -1. E-05	-2.913340 -1. E-05	-3.153322 -1. E-05	1.000134 -1. E-05

TABLE 3.7

SOLUTION OF BOUNDARY VALUES FROM IDENTIFICATION
SHOWN IN TABLE 3.6 WHERE b_1, b_2 and b_3
ARE FIT IN A LEAST SQUARE SENSE AND
SPECIFIED TO 4 SIGNIFICANT DIGITS

i	specified b_i	solution b_i
1	.1992	.1992
2	.0762	.0762
3	.1409	.1409
4	0.0	8. E-11
5	0.0	3. E-11
6	0.0	-1. E-10
7	0.0	2. E-11
8	0.0	-2. E-10
9	0.0	7. E-11
10	0.0	1. E-10

were met.

Heat Conduction Equation

The heat conduction equation

$$\frac{\partial u}{\partial x} = \frac{\partial^2 u}{\partial y^2} \qquad (3.5)$$

with boundary conditions

$$u(x,0) = u(x,1) = 0 \qquad (3.6)$$
$$u(0,y) = \sin \pi y$$

was approximated by substituting a second order central difference operator for $\frac{\partial^2 u}{\partial y^2}$ and integrated with a predictor-corrector integration method. The first results shown in column 1 of Table 3.8 show that the accuracy obtained from a three line approximation is poor. An integration step size of .01 was used. The ratio, $w = \Delta x / \Delta y^2$, was .16 for this integration step size and was held constant as the number of lines increased. The second column contains the results of a seven line approximation again with $w = .16$. There is some improvement in accuracy, but still somewhat less than desirable. The fifteen line approximation proves to be accurate to two or three significant figures.

In Table 3.9 is shown the error in the approximate solutions shown in Table 3.8.

To contrast the second order operator, a higher order

TABLE 3.8

APPROXIMATE SOLUTIONS OF UNSTEADY HEAT CONDUCTION EQUATION USING 2ND ORDER DIFFERENCE OPERATORS

x	y	3 lines	7 lines	15 lines	Analytical
.05	.125	--*	.235	.2339	.2336
.05	.25	.442	.434	.4323	.4317
.05	.5	.626	.614	.6115	.6105
.2	.125	--	.545 E-01	.5350 E-01	.5316 E-01
.2	.25	.108	.100	.9885 E-01	.9822 E-01
.2	.5	.153	.142	.1398	.1389
.4	.125	--	.776 E-02	.7478 E-02	.7384 E-02
.4	.25	.166 E-01	.143 E-01	.1382 E-01	.1364 E-01
.4	.5	.235 E-01	.203 E-01	.1954 E-01	.1930 E-01
1.0	.125	--	.224 E-04	.2043 E-04	.1979 E-04
1.0	.25	.597 E-04	.415 E-04	.3775 E-04	.3657 E-04
1.0	.5	.844 E-04	.586 E-04	.5338 E-04	.5172 E-04
2.0	.125	--	.132 E-08	.1091 E-08	.1024 E-08
2.0	.25	.504 E-08	.243 E-08	.2015 E-08	.1892 E-08
2.0	.5	.713 E-08	.344 E-08	.2850 E-08	.2675 E-08

* no values are available

TABLE 3.9

DIFFERENCE BETWEEN ANALYTICAL AND APPROXIMATE
SOLUTIONS SHOWN IN TABLE 3.8

x	y	3 lines	5 lines	7 lines
.05	.125	--*	-.002	-.0003
.05	.25	-.011	-.002	-.0006
.05	.5	-.016	-.004	-.0010
.2	.125	--	.001	.0003
.2	.25	-.01	.002	.0006
.2	.5	.015	.004	.0001
.4	.125	--	.003 E-01	.0009
.4	.25	.03 E-01	.007 E-01	.0018 E-01
.4	.5	.04 E-01	.010 E-01	.0014 E-01
1.0	.125	--	.027 E-04	.0064 E-04
1.0	.25	.232 E-04	.050 E-04	.0118 E-04
1.0	.5	.327 E-04	.069 E-04	.0166 E-04
2.0	.125	--	.030 E-08	.0067 E-08
2.0	.25	.315 E-08	.054 E-08	.0123 E-08
2.0	.5	.445 E-08	.066 E-08	.0175 E-08

* no values are available

operator was used to approximate $\partial^2 u/\partial y^2$ as was done for
the Laplace equation. A fourth order central difference
operator, Eq. (2.6), was used for the lines not adjoining
a boundary and a special operator shown in Eqs. (2.7) was
used for the lines adjoining a boundary.

A significant increase in accuracy is observed in the
calculations shown in Table 3.10. The ratio, w, was kept
equal to .16 throughout the integration of the higher order
equations. These results show that a good accuracy may be
obtained by use of a reasonable number of lines to approxi-
mate the continuous equations. In Table 3.11 the error in
the approximate solutions in Table 3.10 is shown.

The inverse problem was to identify c in

$$\frac{\partial u}{\partial x} = c \, \frac{\partial^2 u}{\partial y^2} \tag{3.7}$$

with the boundary conditions given in Eq. (3.6). As a
first experiment, one boundary condition was specified at
x = .5. A seven line approximation was used with predictor
corrector integration while maintaining w = .16. The
boundary condition, given at y = .5, was b_1 = .0071919,
which is accurate to five significant digits. This
accuracy was greater than was obtained in the direct
integration with seven lines as shown in Table 3.10. The
constant was identified to four digits of accuracy in seven
iterations as shown in Table 3.12, and the boundary value

TABLE 3.10

APPROXIMATE SOLUTIONS OF UNSTEADY HEAT CONDUCTION EQUATION USING 4TH ORDER DIFFERENCE OPERATORS

x	y	7 lines	15 lines	Analytical
.05	.125	.233527	.233628	.233628
.05	.25	.431635	.431689	.431687
.05	.5	.610504	.610502	.610498
.2	.125	.531247 E-01	.531599 E-01	.531590 E-01
.2	.25	.981923 E-01	.982270 E-01	.982251 E-01
.2	.5	.138884	.138914	.138911
.4	.125	.737756 E-02	.738465 E-02	.738439 E-02
.4	.25	.136362 E-01	.136451 E-01	.136446 E-01
.4	.5	.192871 E-01	.192971 E-01	.192963 E-01
1.0	.125	.197588 E-04	.197956 E-04	.197937 E-04
1.0	.25	.365209 E-04	.365776 E-04	.365740 E-04
1.0	.5	.516544 E-04	.517285 E-04	.517234 E-04
2.0	.125	.012057 E-08	.102400 E-08	.102380 E-08
2.0	.25	.188635 E-08	.189210 E-08	.189173 E-08
2.0	.5	.266806 E-08	.267584 E-08	.267531 E-08

TABLE 3.11

DIFFERENCE BETWEEN ANALYTICAL AND APPROXIMATE
SOLUTIONS SHOWN IN TABLE 3.10

x	y	7 lines	15 lines
.05	.125	.000100	-.000001
.05	.25	.000052	-.000002
.05	.5	-.000006	-.000004
.2	.125	.000024	-.000001
.2	.25	.000033	-.000002
.2	.5	.000027	-.000003
.4	.125	.000068 E-01	-.000002 E-01
.4	.25	.000084 E-01	-.000005 E-01
.4	.5	.000092 E-01	-.000008 E-01
1.0	.125	.000349 E-04	-.000019 E-04
1.0	.25	.000531 E-04	-.000036 E-04
1.0	.5	.000690 E-04	-.000051 E-04
2.0	.125	.000323 E-08	-.000020 E-08
2.0	.25	.000538 E-08	-.000037 E-08
2.0	.5	.000725 E-08	-.000053 E-08

TABLE 3.12

IDENTIFICATION IN UNSTEADY HEAT CONDUCTION
EQUATION FROM ONE BOUNDARY VALUE
CORRECT TO 5 SIGNIFICANT DIGITS

Iteration	c	b	γ
1	.5000	.084790	3.708
2	.6854	.033953	2.330
3	.8451	.015437	1.280
4	.9533	.0090486	4.36 E-01
5	.9949	.0073699	4.92 E-02
6	.99981	.0071940	5.97 E-04
7	.99987	.0071919	4.28 E-08
Analytical	1.00000	.0071919	

TABLE 3.13

IDENTIFICATION IN UNSTEADY HEAT CONDUCTION EQUATION
FROM 10 DATA POINTS CORRECT TO 4 SIGNIFICANT
DIGITS USING LEAST SQUARE FIT

Iter.	c	b_1	b_5	b_{10}	γ
1	.5000	.2989	.1114	.03243	5.8
2	.7933	.2586	.05401	.007626	2.2
3	.9658	.2375	.03528	.003254	3.4 E-01
4	.9986	.2336	.03254	.002768	8.5 E-03
5	.99944	.2336	.03248	.002757	3.3 E-06
Anal.	1.00000	.2336	.03245	.002752	

was satisfied to five digits of accuracy. It may be noted that the constant γ decreased at a quadratic rate and thus the initial condition also converged at a quadratic rate. The execution time required for this identification was 1.8 minutes.

Ten data points were then specified along y = .125 which had been rounded off to four significant digits. In Table 3.13 are shown results using a least square fit of the data. The constant was identified to four digits of accuracy in five iterations, and the boundary conditions were met to different degrees of accuracy. This is easily explained when one realizes that the least square approach minimizes the sum of square of the deviations from the specified boundary conditions and thus the smaller boundary values would not be met as accurately. A weighting procedure would alleviate this problem.

In Table 3.14 are presented the results of a pseudo-least square fit. The results are similar to those of Table 3.13. For this problem there is very little difference in the results of the two types of fit criteria. Table 3.13 shows the difference between the given data and the integrated solutions for the least square and the pseudo-least square fits. There is little difference in the sum of the square of the deviations from the boundary values for the two methods.

TABLE 3.14

PROBLEM SHOWN IN TABLE 3.13 USING
PSEUDO-LEAST SQUARE FIT

Iteration	c	b_1	b_5	b_{10}	γ
1	.5000	.2989	.1114	.03243	6.7
2	.8362	.2531	.04859	.006171	1.7
3	.9841	.2354	.03372	.002973	1.5 E-01
4	.9992	.2336	.03249	.002760	1.2 E-03
5	.99935	.2336	.03248	.002758	-1.2 E-07
Anal.	1.00000	.2336	.03245	.002752	

TABLE 3.15

COMPARISON OF LEAST SQUARE WITH PSEUDO-LEAST
SQUARE FIT FOR DATA SHOWN IN
TABLES 3.13 AND 3.14

i	pseudo least square $-b_i$*	least square $-b_i$*
1	2.0 E-06	-1.0 E-05
2	-6.0 E-05	-7.0 E-05
3	3.8 E-05	2.7 E-05
4	3.2 E-05	2.3 E-05
5	3.2 E-05	3.0 E-05
6	2.5 E-05	2.0 E-05
7	2.0 E-06	2.0 E-06
8	12.2 E-06	9.9 E-06
9	8.6 E-06	6.9 E-06
10	6.1 E-06	4.9 E-06

*specified boundary condition to be met

Another set of calculations was made using the same ten boundary conditions used in Table 3.13 and 3.14 except that the boundary conditions were correct to only two significant figures. The constant c was identified to two significant figures as shown in Table 3.16 in five iterations.

Poisson Equation

A nine line approximation was used to solve

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = J_0(2_3 r) \tag{3.8}$$

in the domain of the unit square with the boundary conditions given in Eq. (2.36). A fourth order central difference operator was substituted for lines n = 2 through n = 8 and second order forward and backward difference operators for lines n = 1 and n = 9, respectively.

$$E^2(U_1) = (-U_4 - 4U_3 - 5U_2 - 2U_1)/\Delta y^2$$

$$E^2(U_9) = (2U_9 - 5U_8 - 4U_7 - U_6)/\Delta y^2$$

The results are shown in Tables 3.17 and 3.18 and compared to the analytical solution. The approximation was accurate to three and four significant figures within the unit circle.

TABLE 3.16

IDENTIFICATION IN UNSTEADY HEAT CONDUCTION EQUATION FROM 10 DATA POINTS CORRECT TO 2 SIGNIFICANT DIGITS USING PSEUDO-LEAST SQUARE FIT

Iteration	c	b_1	b_5	b_{10}	γ
1	.5000	.2989	.1114	.03243	6.8
2	.8425	.2524	.04783	.005981	1.8
3	.9995	.2336	.03247	.002519	3.0 E-03
4	1.0179	.2315	.03102	.002516	2.2 E-05
Analytical	1.0000	.2336	.03245	.002752	
Specified Data		.2300	.03200	.002800	

TABLE 3.17

COMPARISON OF APPROXIMATE AND ANALYTICAL SOLUTIONS OF POISSON
EQUATION USING 4TH ORDER DIFFERENCE OPERATORS

x	U_1	U_2	U_3	U_4	U_5
.0000	.015284	.010853	.006044	.001632	.000000
*	.015765	.011339	.005942	.001634	.000000
.0159	.015009	.010017	.004664	.000000	-.001740
*	.015325	.010426	.004601	.000000	-.001740
.0670	.013665	.006967	.000000	-.005550	-.007629
*	.013636	.007190	.000000	-.005552	-.007629
.0870	.012984	.005672	-.001898	-.007805	-.010026
*	.012871	.005833	-.001889	-.007807	-.010026
.1693	.009680	.000000	-.009830	-.017199	-.019914
*	.009423	.000000	-.009830	-.017192	-.019926
.2793	.004950	-.007312	-.019564	-.028578	-.031874
*	.004764	-.007378	-.019598	-.028589	-.031881
.5000	.000000	-.014567	-.028936	-.039391	-.043225
*	.000000	-.014616	-.028960	-.039410	-.043238

*The second line for each value of x is the exact solution.

TABLE 3.18

CONTINUATION OF TABLE 3.17

x	U_1	U_2	U_3	U_4	U_5
.5800	.000712	-.013530	-.027611	-.037887	-.041631
*	.000682	-.013595	-.027655	-.037905	-.041643
.6800	.003412	-.009594	-.022547	-.032027	-.035491
*	.003277	-.009664	-.022577	-.032031	-.035500
.8307	.009680	.000000	-.009831	-.017199	-.019914
*	.009423	.000000	-.009829	-.017192	-.019926
.9330	.013665	.006967	.000000	-.005550	-.007629
*	.013636	.007190	.000000	-.005552	-.007629
.9730	.014769	.009385	.003679	-.001171	-.002986
*	.014981	.009749	.003637	-.001174	-.002986
.9841	.015009	.010017	.004664	.000000	-.001740
*	.015325	.010426	.004601	.000000	-.001740
1.0000	.015284	.010853	.006044	.001632	.000000
*	.015765	.011339	.005942	.001634	.000000

*The second line for each value of x is the exact solution

Mildly Nonlinear Equation

The problem

$$u_{xx} + u_{yy} = e^u \qquad (3.9)$$

was considered over a rectangular domain, $0 \leq x \leq .5$ and $0 \leq y \leq .25$ with

$$u(S) = 0$$

where S is the boundary of the domain. A seven line approximation was used with fourth order difference operators for u_{yy}.

The solution presented some problems because e^u could not be calculated by the standard library subroutine if $u > 173$. Thus a method similar to an imbedding procedure was incorporated into the program. The integration was continued until dU_i/dx became larger than some number z which was arbitrarily chosen as 170. When this occurred, say at x_1, the integration was stopped and the initial conditions were found which would satisfy the boundary conditions at x_1. The problem was integrated again, and if the derivative became greater than z, the procedure was repeated.

It was found that this iteration of similar boundary value problems did not always converge. The procedure would reach a given point x_1 and not continue to the specified boundary. However, when the integration step

size, $\triangle x$, was reduced to a certain value, the procedure converged.

In Table 3.1) are shown the solutions of Eq. (3.9) for four representative points in the domain. The results in column 1 and 3 were obtained by integrating along lines in the x direction, while column 1 and 4 were integrated along lines in the y direction. The results obtained in all four cases required the use of the iteration of similar boundary value problems. For a seven line approximation with lines in the x direction and using a four order set of operators for $E^2(U_i)$, it was found that the iteration of similar boundary values did not converge for a step size equal to or greater than .0025 in a fourth order Runge-Kutta scheme.

The numerical integration of Eq. (3.9) has also been considered by Bellman and Kalaba [6] and Greenspan [29]. From the information given in [6], it is difficult to make any conclusions comparing the methods.

TABLE 3.19

APPROXIMATE SOLUTION OF MILDLY NONLINEAR EQUATION
AT FOUR REPRESENTATIVE POINTS IN THE DOMAIN

x	y	$u_1(x,y)$	$u_2(x,y)$	$u_3(x,y)$	$u_4(x,y)$
.0625	.125	-.004547	-.004575	-.0046017	-.0046020
.125	.125	-.005968	-.0060345	-.0060396	-.0060402
.0625	.25	-.005298	-.0053396	-.0053396	-.0053399
.125	.25	-.007020	-.0070778	-.0070778	-.0070785

$u_1(x,y)$ = 2nd Order Approximation with three continuous
lines in the y direction. $0 \leq y \leq .5$

$u_2(x,y)$ = 4th Order approximation with seven continuous
lines in the x direction. $0 \leq x \leq .25$

$u_3(x,y)$ = 4th Order approximation with seven continuous
lines in the y direction. $0 \leq y \leq .5$

$u_4(x,y)$ = 4th Order approximation with fifteen continuous
lines in the x direction. $0 \leq x \leq .25$

CHAPTER IV

SUMMARY, DISCUSSION, CONCLUSIONS AND RECOMMENDATIONS

Summary

A method of solving a class of inverse problems known as identification problems has been described for partial differential equations. The procedure employs the method of lines for approximation of the partial differential equation and the Newton-Raphson-Kantorovich expansion in function space which reduces the solution for nonlinear equations to an iterative process of solving linear equations.

The method of lines with the superposition of particular solutions was shown to be an effective method of numerically solving linear boundary value problems. By the use of the linearization procedure, the identification problem and the nonlinear partial differential equations were reduced to successively solving linear boundary value problems.

The general procedure was numerically illustrated for the Laplace equation, a Poisson equation, an unsteady heat conduction equation, and a mildly nonlinear equation.

Discussion and Recommendations for Further Work

The identification procedure proved to be stable in

both examples considered, and the constant was identified to the same accuracy as the data. This indicates that the solution of the partial differential equations was sensitive to the constant parameters to be identified. This sensitivity is an important factor in any identification process.

The Laplace equation integrated as an initial value problem and the solution of the unsteady heat conduction equation for negative time are both examples of ill-posed problems. The Laplace equation is sensitive to initial derivatives which led to its ill-posed nature and exhibited itself in instability of numerical integration. The unsteady heat conduction equation is insensitive to initial values of the function and thus can lead to an ill-posed problem if it is desired to identify the initial value of the function from data within the domain. The ill-posed nature is exemplified by the resulting ill-conditioned matrix to be inverted. It was shown that the possibility of the ill-posed nature did not interfere with the identification. Further work needs to be done in the area of inverse problems associated with diffusion type equations.

In this dissertation the Jacobian matrix associated with the linearization process was evaluated analytically. However, some indication has been given [38,39] that this evaluation might be done numerically. It is not entirely clear though how this would affect the required computation

time or the stability of the process.

Another improvement which can be made and should be investigated is the use of different higher order operators for approximating the derivatives with respect to all but one of the independent variables. These operator approximations lead to the truncation error, which was the dominate error in the procedure of identification. Boyd [24] has used some best fit operators which are designed to control the noise introduced by this approximation. Again, further investigation should be directed along these lines to make the approximation method more effective.

A problem inherent in the Newton-Raphson-Kantorovich linearization procedure is the convergence space of initial approximation. This convergence space did not present many problems for the equations considered in this dissertation. However, it is conceivable that such problems will arise and the methods discussed in Appendix C might be incorporated to increase the convergence space. Another possibility is to employ gradient techniques to get an approximation which is within the convergence space. The method of "similar boundary value problems" was used to solve two point boundary value problems in which the nature of the problem and/or the integration scheme is unstable. An investigation should be done to extend this method to multipoint boundary value problems.

Conclusions

The identification procedure was shown to be effective for the equations,

$$u_{xx} + c\, u_{yy} = 0$$
$$u_t - c\, u_{xx} = 0$$

The integration procedure was also shown to give good results for the following boundary value problems:

$$u_{xx} + u_{yy} = f(x,y)$$
$$u_{xx} + u_{yy} = e^u$$

The method was shown to identify the parameters in these equations to the same accuracy as the data.

The method of reduction and integration procedure is easily programed and provides an effective way of solving both linear and nonlinear partial differential equations.

Dimensionality might be critical for some problems, but this is inherent in most numerical methods for solution of boundary value problems in partial differential equations. However, it is not as big a problem in this method as it is in other general methods.

The method is easy to program. It is assumed that the program developed by Holloway and Childs and described by Holloway [11] is available. The method then requires a programming effort comparable to that required to solve an initial value problem using a documented forward integration

scheme. Generally it requires preparation of one data card
for each irregular boundary value in addition to a few
information data cards. The method requires less program-
ming effort to adapt to a new problem, probably less
computer time to solve a given problem to an arbitrary high
accuracy, and yields the most explicit indication of
accuracy of most and possibly all general methods for the
numerical solution of multipoint boundary value problems,
in linear and nonlinear partial differential equations
within arbitrary boundaries, presently known to the author.
Thus, extension to more difficult problems than the simple
examples used is merely a matter of programming and
computer time.

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APPENDIX A

DEFINITION OF TERMS

In this appendix is presented the definitions of some terms which appear in the dissertation and should be defined for the clarity of the presentation.

Differential-difference equations. This refers to those equations which arise from substitution of difference operators for differential operators and have two or more independent variables with differentiation with respect to one and differencing with respect to the others [30] pg. 127.

Unstable. The numerical integration of a differential equation will be termed "unstable" if for a given set of initial conditions and a step size, h, the solution diverges from the solution of the differential equation as the integration proceeds [31] pg. 147.

Mildly nonlinear. The elliptic equation

$$u_{xx} + u_{yy} + u_{zz} = F(x, y, z, u_x, u_y, u_z)$$

is said to be "mildly nonlinear" if

$$\frac{\partial F}{\partial u} > 0$$

and

$$\frac{\partial F}{\partial u_x}, \ \frac{\partial F}{\partial u_y}, \ \frac{\partial F}{\partial u_z} \quad \text{are bounded}$$

Under sufficiently strong smoothness hypotheses, a "mildly nonlinear" Dirichlet problem has a unique solution [29].

<u>Quasilinear</u> <u>ordinary</u> <u>differential</u> <u>equation</u>. An
equation in which the highest order derivative appears
linearly.

<u>Spurious</u> <u>roots</u>. If a differential equation is
approximated by a difference equation of higher order than
the corresponding differential equation, then spurious
(or extra) solutions arise. The roots corresponding to
these spurious solutions are known as "spurious roots."

APPENDIX B

SUPERPOSITION OF PARTICULAR SOLUTIONS

From the classical theory of ordinary differential equations, it is known that the solution of an nth order linear ordinary differential equation is a linear combination of n independent solutions of the homogeneous differential equation plus a particular solution of the complete differential equation. This appendix will demonstrate that an additional condition is required in order to use superposition of particular solutions to satisfy the complete equation and the boundary conditions.

Consider the following system of linear first order differential equations

$$\frac{d\overline{V}}{dx} = A\overline{V} + \overline{B}$$

(B.1)

where A is an n x n matrix which may be a function of x. Let

$$\overline{V} = \Phi_p \overline{\gamma}$$

(B.2)

and

$$\sum_{i=1}^{n+1} \gamma_i = 1$$

(B.3)

where Φ_p is a matrix of solutions of Eq. (B.1) of which n are independent and therefore Φ_p is of rank n.

$$\Phi_p = \left[\overline{P}_1 \mid \overline{P}_2 \mid \cdot \cdot \cdot \mid \overline{P}_{n+1} \right]$$

and

$$\overline{\gamma} = \left[\gamma_1 \mid \gamma_2 \mid \cdots \mid \gamma_{n+1} \right]^T$$

Thus Φ_p satisfies the differential equation

$$\frac{d\Phi_P}{dx} = A\Phi_P - D \tag{B.4}$$

where D is an ($n \times n+1$) matrix

$$D = \left[\overline{B} \mid \overline{B} \mid \cdots \mid \overline{B} \right]$$

To show that Eq. (B.2) is the solution together with Eq. (B.3), it is necessary that it satisfy Eq. (B.1). Substituting Eq. (B.2) into Eq. (B.1)

$$\frac{d\Phi_P}{dx}\overline{\gamma} = A\Phi_P\overline{\gamma} + \overline{B} \tag{B.5}$$

Subtracting $D\overline{\gamma}$ from both sides of Eq. (B.5) and rearranging terms,

$$\left(\frac{d\Phi_P}{dx} - A\Phi_P - D \right)\overline{\gamma} = \overline{B} - D\overline{\gamma} \tag{B.6}$$

By Eq. (B.4) the left side of Eq. (B.6) is identically the null vector and therefore

$$D\overline{\gamma} = \overline{B}$$

which gives

$$B_j \sum_{i=1}^{n+1} \gamma_i = B_j \qquad 1 \leq j \leq n$$

or

$$\sum_{i=1}^{n+1} \gamma_i = 1$$

which is the condition given in Eq. (B.3).

If the initial conditions are chosen such that $\overline{P}_{n+1}$ satisfies the boundary conditions, then

$$\overline{P}_{n+1} = \Phi_P' \, \overline{\gamma}' + \overline{P}_{n+1} \, \gamma_{n+1} \tag{B.6}$$

where Φ_P' is a submatrix of Φ_P

$$\Phi_P = \left[\, \Phi_P' \mid \overline{P}_{n+1} \, \right]$$

and

$$\overline{\gamma} = \left[\frac{-\overline{\gamma}'}{\gamma_{n+1}} \right]$$

Solving for γ_{n+1} in Eq. (B.3) and substituting into Eq. (B.6) gives

$$\overline{P}_{n+1} = \Phi_P' \, \overline{\gamma}' + \overline{P}_{n+1} - \overline{P}_{n+1} \sum_{i=1}^{n} \gamma_i$$

which reduces to

$$0 = \left[\, \overline{P}_1 - \overline{P}_{n+1} \mid \overline{P}_2 - \overline{P}_{n+1} \mid \cdots \mid \overline{P}_n - \overline{P}_{n+1} \, \right] \overline{\gamma}'$$

It will be shown that

$$\det \left[\, \overline{P}_1 - \overline{P}_{n+1} \mid \overline{P}_2 - \overline{P}_{n+1} \mid \cdots \mid \overline{P}_n - \overline{P}_{n+1} \, \right] \neq 0$$

by proper choice of the initial matrix $\Phi_P(x_o)$ where x_o is the initial value of x.

Thus $$\overline{\gamma}' = 0$$

and $$\gamma_{n+1} = 1 \tag{B.7}$$

The rank of the initial matrix, $\Phi_p(x_o)$, must be n. We denote by $\overline{\alpha}$ the vector which represents the initial conditions of the solution $\overline{P}_{n+1}$. We introduce an array Q

such that

$$\rho_i \neq 0 \qquad 1 \leq i \leq n$$

We now take the initial matrix to be

$$\Phi_p(x_0) = \begin{bmatrix} \alpha_1 + \rho_1 & \alpha_1 & \cdot & \cdot & \cdot & \alpha_1 & \alpha_1 \\ \alpha_2 & \alpha_2 + \rho_2 & \cdot & \cdot & \cdot & \alpha_2 & \alpha_2 \\ \alpha_3 & \alpha_3 & \cdot & \cdot & \cdot & \alpha_3 & \alpha_3 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \alpha_n & \alpha_n & \cdot & \cdot & \cdot & \alpha_n + \rho_n & \alpha_n \end{bmatrix}$$

By successively subtracting the last column from each of the other columns, etc., we get the normal form of this matrix to be a diagonal matrix with diagonal elements ρ_i. Thus, $\Phi_p(x)$ is obviously of rank n.

With this choice of initial conditions, the constants are related directly to the new initial conditions.

$$\overline{V}(x_0) = \Phi(x_0)\overline{\gamma}$$

or

$$V_i(x_0) = \alpha_i \sum_{j=1}^{n+1} \gamma_j + \gamma_i \rho_i$$

Substituting the constraint condition Eq. (B.3) gives

$$V_i(x_0) = \alpha_i + \gamma_i \rho_i \qquad (B.8)$$

It is obvious then that

$$\rho_i \gamma_i / \alpha_i = (V_i(x_0) - \alpha_i)/\alpha_i \qquad (B.9)$$

Equation (B.9) shows the relative change in the initial

condition vector if the solution $\bar{P}_{n+1}$ does not satisfy the boundary conditions. We have found by experience that the values ϱ_i can often be quite arbitrary, but, in some cases it is advantageous to use

$$\varrho_i = \beta \alpha_i$$

where generally

$$10^{-10} < |\beta| < 1$$

and α_i must be nonzero. If α_i is near zero, we use arbitrary scalars for ϱ_i.

Theoretically, the solution of a linear problem can be solved with a one pass algorithm. However, roundoff error often prevents this in numerical applications. Thus, we suggest that even linear problems be solved iteratively with the above scheme.

The work shown in this appendix follows Childs [32] and Holloway [11] and has since appeared in part in an independent investigation reported by Miele [33].

In summary, it has been shown that linear boundary value problems can be solved by superposition of particular solutions with an additional constraint equation. The following observations are of importance:

1. The matrix to be inverted is never singular. This is ensured by the proper choice of initial conditions. Apparently, Miele [33] pg. 265, had trouble with this.

2. In an application, the goodness of satisfaction

of Eq. (B.7) together with Eq. (B.9) is an explicit
indication of the roundoff error existing in the numerical
method of solution.

This latter observation was not reported by Miele. We
do agree with the positive observations of Miele.

APPENDIX C

NEWTON-RAPHSON-KANTOROVICH EXPANSION IN FUNCTION SPACE

The Newton's method for functional equations has been often referred to as the Newton-Raphson-Kantorovich expansion in function space [6] pg. 22. The method is very important because it is one of the few practical methods available at the present time for finding the actual solution of a non-linear functional equation [34] pg. 695. The theory of this method is based on the theory of functional analysis and no attempt will be made in this appendix to show the convergence properties which are generally shown through the theorems developed in functional analysis or through their relation to the theory dynamic programming with its concept of approximation in policy space. Convergence proofs may be found in Kalaba [34] and Kantorovich and Akilov [35].

In this dissertation the linearization procedure was carried out within the framework of the ordinary differential equations. However, this expansion may also be carried out directly for partial differential equations.

As a first example, consider the second order quasi-linear partial differential equation considered by Kantorovich

$$A u_{xx} + B u_{xy} + C u_{yy} + D = 0 \qquad \text{(c.1)}$$

Let

$$P(u) = A u_{xx} + B u_{xy} + C u_{yy} + D \qquad (C.2)$$

where A, B, C and D are functions of x, y, u, u_x, and u_y.
Assume u^{k+1} to be the solution. Expand Eq. (C.1) about
the solution u^{k+1}

$$0 = \left.\frac{\partial P(u)}{\partial u}\right|^k (u^{k+1} - u^k) + \left.\frac{\partial P(u)}{\partial u_x}\right|^k (u_x^{k+1} - u^k)$$

$$+ \left.\frac{\partial P(u)}{\partial u_y}\right|^k (u_y^{k+1} - u_y^k) + \left.\frac{\partial P(u)}{\partial u_{xx}}\right|^k (u_{xx}^{k+1} - u_{xx}^k) \qquad (C.3)$$

$$+ \left.\frac{\partial P(u)}{\partial u_{yy}}\right|^k (u_{yy}^{k+1} - u_{yy}^k) + \left.\frac{\partial P(u)}{\partial u_{xy}}\right|^k (u_{xy}^{k+1} - u_{xy}^k) + P^k(u)$$

For Eq. (C.1)

$$\left.\frac{\partial P}{\partial u_{yy}}\right|^k = A^k, \quad \left.\frac{\partial P}{\partial u_{xy}}\right|^k = B^k, \quad \left.\frac{\partial P}{\partial u_{yy}}\right|^k = C^k \qquad (C.4)$$

$$\left.\frac{\partial P}{\partial u}\right|^k = \left(\frac{\partial A}{\partial u} u_{xx} + \frac{\partial B}{\partial u} u_{xy} + \frac{\partial C}{\partial u} u_{yy} + \frac{\partial D}{\partial u}\right)^k = d_1^k \qquad (C.5)$$

$$\left.\frac{\partial P}{\partial u_x}\right|^k = \left(\frac{\partial A}{\partial u_x} u_{xx} + \frac{\partial B}{\partial u_x} u_{xy} + \frac{\partial C}{\partial u_x} u_{yy} + \frac{\partial D}{\partial u_x}\right)^k = d_2^k \qquad (C.6)$$

$$\left.\frac{\partial P}{\partial u_y}\right|^k = \left(\frac{\partial A}{\partial u_y} u_{xx} + \frac{\partial B}{\partial u_x} u_{xy} + \frac{\partial C}{\partial u_y} u_{yy} + \frac{\partial D}{\partial u_y}\right)^k = d_3^k \qquad (C.7)$$

Thus by Eq. (C.4)

$$\left.\frac{\partial P}{\partial u_{xx}}\right|^k u_{xx}^k + \left.\frac{\partial P}{\partial u_{xy}}\right|^k u_{xy}^k + \left.\frac{\partial P}{\partial u_{yy}}\right|^k u_{yy}$$

$$= P^k(u) - D^k \qquad (C.8)$$

Eq. (C.3) then reduces to the linearized equation

$$(A^k u_{xx}^{k+1} + B^k u_{xy}^{k+1} + C^k u_{yy}^{k+1} + D^k) +$$

$$+ (d_1^k u^{k+1} + d_2^k u_y^{k+1} + d_3^k u_y^{k+1})$$

$$- (d_1^k u^k + d_2^k u^k + d_3^k u^k) = 0$$

Let
$$P'[u^k](u^{k+1}) = A^k u_{xx}^{k+1} + B u_{xy}^{k+1} + C^k u_{yy}^{k+1}$$

$$+ d_1^k u^{k+1} + d_2^k u_x^{k+1} + d_3^k u_x^{k+1}$$

Thus, with the operator, P, notation the quasilinear equation

$$P(u) \overset{d}{=} P[u](u) = 0 \qquad (C.9)$$

is reduced to the solution of the linear equations

$$P'[u^k](u^{k+1} - u^k) + P[u^k](u^k) = 0$$
$$K = 1, 2, \cdots \qquad (C.10)$$

The necessary conditions for such an expansion is that

$$\frac{\partial P}{\partial u}, \quad \frac{\partial P}{\partial u_x}, \quad \frac{\partial P}{\partial u_y}$$

be continuous and that u^0 be sufficiently close to u^*, where u^* is the solution, so that the expansion Eq. (C.10) is valid.

Consider a set of nonlinear ordinary differential equations which are written as a nonlinear first order vector differential equation

$$\frac{d\overline{u}}{dx} = f(\overline{u}, x) \qquad (C.11)$$

The linearized equation is

$$\frac{d\overline{u}}{dx}^{k+1} = f(\overline{u}^k, x) + \frac{\partial f}{\partial \overline{u}}\bigg|^k (\overline{u}^{k+1} - \overline{u}^k) \qquad (C.12)$$

One problem which is often associated with Newton's method is finding an initial estimate of u^o which is close enough to u^* to give a convergence sequence of functions $\{u^k\}$ $k = 1, 2, \ldots$

Two methods have been used in our studies to extend the convergence space. The first method is a modification of Eq. (B.7)

$$\alpha_i^{k+1} = \alpha_i^k + (1-\sigma)\, \gamma_i\, \alpha_i^k\, \beta \tag{C.13}$$

where γ_i is the ith constant from Eq. (2.25), α_i^k is the estimate for the ith unknown initial condition on the kth iteration, σ is a damping factor which is a function of k such that $0 \le \sigma(k) \le 1$. If $\sigma = 0$, then Eq. (C.13) is identical with Eq. (B.7). If σ is close to 1, then there will be little difference between α_i^{k+1} and α_i^k as long as γ_i and β are not too large. With $\sigma \neq 0$, one could not expect quadratic convergence and Eq. (C.13) would be related to gradient type algorithms. This modification and some similar such modifications have been considered by Breakwell, et al [35], Lastman [36] and Paine [12].

Another modification is to use apriori knowledge concerning the missing initial conditions. This apriori knowledge is to place limits on the missing initial conditions. Again, this may interfere with the quadratic convergence, but increases the convergence space.

APPENDIX D

SOLUTION OF LAPLACE EQUATION BY METHOD OF LINES

This appendix presents the analytical solution of the "method of lines" approximation to the Laplace equation with boundary conditions

$$u(1,y) = u(x,0) = u(x,1) = 0 \qquad (D.1)$$
$$u(0,y) = \sin \pi y$$

This equation is approximated by a set of lines in the x direction and a second order central difference operator is substituted for $\partial^2 u / \partial y^2$.

$$\frac{d^2 U_m}{dx^2} + (U_{m+1} - 2U_m + U_{m-1})/h^2 = 0 \qquad (D.2)$$
$$1 \leq m \leq n$$

Assuming a solution of the form

$$U_m(x) = \varrho(m)\, v(x)$$

gives

$$\varrho(m) \frac{d^2 v}{dx^2} + (\varrho(m+1) - 2\varrho(m) + \varrho(m-1))v/h^2 = 0$$

or

$$\frac{d^2 v}{dx^2}/v = -(\varrho(m-1) - 2\varrho(m) + \varrho(m-1))/h^2 \varrho(m) = \delta^2$$
$$1 \leq m \leq n$$

To find $\varrho(m)$ we solve the homogeneous difference equation

$$\varrho(m-1) - (2 - h^2 \delta^2)\varrho(m) + \varrho(m-1) = 0 \qquad (D.3)$$

with boundary conditions

$$\varrho(0) = \varrho(n+1) = 0$$

The general solution of the difference equation, Eq. (D.3), is

$$\rho(m) = C_1 \lambda_1^m + C_2 \lambda_2^m$$

where C_1 and C_2 are arbitrary constants and λ_1 and λ_2 are roots of the characteristic equation

$$\lambda^2 - (2 - h^2 \delta^2) \lambda + 1 = 0$$

From boundary conditions Eq. (D.1) we have

$$\rho(0) = C_1 + C_2 = 0 \qquad \text{or} \qquad C_2 = -C_1$$

$$\rho(n+1) = C_1 \lambda_1^{n+1} + C_2 \lambda_2^{n+1} = C_1 (\lambda_1^{n+1} - \lambda_2^{n+1}) = 0$$

Hence,

$$\left(\frac{\lambda_1}{\lambda_2}\right)^{n+1} = 1 \quad \text{or} \quad \frac{\lambda_1}{\lambda_2} = (1)^{\frac{1}{n+1}} = e^{\frac{2\pi i s}{n+1}}$$

$$s = 1, 2, \cdots, n$$

But since $\lambda_1 \lambda_2 = 1$, it follows that

$$\lambda_1^2 = e^{\frac{2\pi i s}{n+1}} \quad , \quad \lambda_2 = \frac{1}{\lambda_2} = e^{\frac{\pi i s}{n+1}}$$

thus

$$\rho_s(m) = C_1 \left(e^{\frac{\pi i s m}{n+1}} - e^{-\frac{\pi i s m}{n+1}} \right)$$

Substituting Eq. (D.4) into Eq. (D.3)

$$\delta^2 = - \frac{\sin \frac{\pi s(m+1)}{n+1} - 2 \sin \frac{\pi s m}{n+1} + \sin \frac{\pi s(m-1)}{n+1}}{h^2 \sin \frac{\pi s m}{n+1}}$$

$$= - \frac{2 \sin \frac{\pi s m}{n+1} \left(\cos \frac{\pi s}{n+1} - 1 \right)}{h^2 \sin \frac{\pi s m}{n+1}} \qquad (D.5)$$

$$= 2 (1 - \cos(\pi s / n+1)) / h^2 = 4 \sin^2 \frac{\pi (y_s - y_0)}{2\ell} / h^2$$

In addition

$$\rho_s(m) = C \sin \frac{\pi s m}{n+1} = C \sin \frac{\pi s (y_m - y_0)}{\ell}$$

Solving the second equation arising from the separation of variables

$$v_s(x) = A_s e^{\delta_s x} + B_s e^{-\delta_s x}$$

The solution of Eq. (D.2) is a combination of the linearly independent solutions

$$U_{m,s}(x) = (A_s e^{\delta_s x} + B_s e^{-\delta_s x}) \sin \frac{\pi s (y_m - y_0)}{\ell}$$

$$U_m(x) = \sum_{s=1}^{n} \sin \frac{\pi s}{\ell} (y_m - y_0)(A_s e^{\delta_s x} + B_s e^{-\delta_s x})$$

where A_s and B_s are arbitrary constants. These constants are found by imposing the remaining boundary conditions

$$U_m(0) = \sin \frac{m\pi}{n+1}$$
$$U_m(1) = 0$$

The solution is found to be

$$U_1 = U_3 = \frac{\sqrt{2}}{2} (\cosh 3.0611 x - \frac{\cosh 3.0611}{\sinh 3.0611} \sinh 3.0611 x)$$

$$U_2 = \frac{2}{\sqrt{2}} U_1$$

By comparing this solution with the analytical solution Eq. (3.3) it is obvious that they differ only by the eigenvalue 3.0611 instead of π.

It may be shown that eigenvalues approach those of the continuous problem as the n, the number of lines, is increased. From Eq. (D.5)

$$\delta_s(h) = \frac{2}{h} \sin \frac{\pi s h}{2\ell} \qquad 1 \leq s \leq n$$

It is necessary to apply l'Hopital's rule to find the limit as $h \to 0$

$$\lim_{h \to 0} \frac{d \delta_s(h)}{dh} = \left(\frac{s\pi}{\ell} \cosh \frac{\pi s h}{2\ell} \right)_{h=0}$$

$$= \frac{s\pi}{\ell} \qquad 1 \leq s \leq n$$

Thus, in the limit, the eigenvalues coincide with the eigenvalues of the continuous problem.

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13. ABSTRACT

A procedure for identification in partial differential equations is described and illustrated by the Laplace equation and the unsteady heat conduction equation. The procedure for solution involves the substitution of difference operators for the partial derivatives with respect to all but one of the independent variables. The linear boundary value problem is solved by superposition of particular solutions. For non-linear boundary value problems which arise from the original form of the equation or from the identification procedure, a Newton-Raphson-Kantorovich expansion in function space is used to reduce the solution to an iterative procedure of solving linear boundary value problems.

For the problems considered, this procedure has proven to be effective and results in a reasonable approximation to the solution of the boundary value problem in partial differential equations. For the identification problem, it is shown that the constant parameters are identified to the same accuracy as the supplementary data used in the identification procedure.