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Dean
THE CONVERGENCE OF A NON-LINEAR PARABOLIC
PARTIAL DIFFERENTIAL EQUATION

BY

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A THESIS

Submitted to the Faculty of the Graduate School of the
Creighton University in Partial Fulfillment of
the Requirements for the Degree of Master
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This thesis is concerned with the application of Newton's method for multi-variable nonlinear functions to the nonlinear partial differential equation which describes two-dimensional flow of gas through porous media.

Newton's method has been shown to be general enough to be applied to other multi-dimensional nonlinear problems. It has been shown to be convergent for at least a practical range of variables and within this range has an extremely rapid rate of convergence. The results obtained from the technique compare quite favorably with other accepted techniques for solving multi-dimensional nonlinear problems. Finally, an approach for a priori convergence prediction is presented with suggestions for further study in this area.
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CHAPTER I

INTRODUCTION

Many equations that describe physical phenomena are nonlinear. Certain forms of these equations have not yet been solved analytically, but with the advent of large computers have been solved numerically.

This paper is concerned with the application of one numerical technique to the solution and the convergence study of one of these nonlinear equations. The technique is Newton's method for multi-variable nonlinear functions [3]. The particular physical system is the nonlinear partial differential equation which describes two dimensional flow of gas through porous media. The general form of the partial differential equation is:

\[
\frac{\partial}{\partial x} \left[ A(\phi(x,y,t),x,y) \frac{\partial}{\partial x} [\phi(x,y,t)] \right] + \frac{\partial}{\partial y} \left[ B(\phi(x,y,t),x,y) \frac{\partial}{\partial y} [\phi(x,y,t)] \right] \\
+ C(x,y) = \frac{\partial}{\partial t} [D(\phi(x,y,t),x,y) \phi(x,y,t)] . \tag{I-1}
\]

Two dimensional numerical models that describe the transient flow of gas through porous media have been in existence for some time. To date the standard technique for solving (I-1) has been the Alternating-Direction Implicit Procedure (ADIP) developed
by Peaceman and Rachford [10]. Other techniques available are
the purely explicit and purely implicit procedures [5,10]. A new
method, the Alternating-Direction Explicit Procedure (ADEP), has
recently been applied to the solution of nonideal gas flow in
porous media by Carter [1] and Quon, et al., [9]. The merits of
this method are still under discussion.

Some of the above methods have features which make them
impractical to use in two dimensional modeling. A brief explana­
tion of the most widely used procedures now follows. First, let
us define:

\[
\frac{\partial f}{\partial s} \approx \Delta^2 s \left( f_{i,j} \right)_{j,n} = \left[ \frac{f_{i+1/2} (g_{i+1} - g_i) - f_{i-1/2} (g_i - g_{i-1})}{\Delta s^2} \right]_{j,n}
\]

(I-2)

\[
\frac{\partial Dg}{\partial t} \approx D \left( \frac{g_{n+1} - g_n}{\Delta T} \right)_{i,j}
\]

(I-3)

where:

\[
i = 0,1,2,\ldots,N+1,
\]

\[
j = 0,1,2,\ldots,M+1,
\]

\[
n = 0,1,\ldots,T.
\]

Common boundary and initial conditions used in conjunction
with equation (I-1) are:
\[
\frac{\partial \phi (x,y,t)}{\partial x} = \frac{\partial \phi (N,y,t)}{\partial x} = \frac{\partial \phi (x,1,t)}{\partial y} = \frac{\partial \phi (x,M,t)}{\partial y} = 0. \quad (I-4)
\]

\[\phi (x,y,0) \text{ is known.} \quad (I-5)\]

Expressing (I-4) in common difference form, one obtains:

\[
\begin{align*}
\frac{\phi_{0,j,n} - \phi_{2,j,n}}{\Delta x} &= \frac{\phi_{N-1,j,n} - \phi_{N+1,j,n}}{\Delta x} = \frac{\phi_{i,0,n} - \phi_{i,2,n}}{\Delta y} = \\
\frac{\phi_{i,M-1,n} - \phi_{i,M+1,n}}{\Delta y} &= 0. \quad (I-6)
\end{align*}
\]

Purely Explicit Procedure

Applying difference equations (I-2) and (I-3) to the general partial differential equation (I-1) and then solving for \( \phi_{i,j,n+1} \), one obtains the following differential equation:

\[
\phi_{i,j,n+1} = \frac{\Delta T}{D_{i,j,n}} \left( \Delta^2_x (A \phi_{i,j,n}) + \Delta^2_y (B \phi_{i,j,n}) + C_{i,j} + \left( \frac{\Delta \phi_{i,j,n}}{\Delta T} \right) \right). \quad (I-7)
\]

By using the purely explicit technique on equations (I-5), (I-6) and (I-7), one solves for the unknowns, \( \phi_{i,j,n+1} \), explicitly. One of its prime limitations is the restriction on the size of the \( \Delta T \) increment. The \( \Delta T \) restriction which is necessary for numerical stability is given by the following relationship:

\[
\frac{\Delta T}{D_{i,j,n}} \left( \frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} \right) \leq 1/4. \quad (I-8)
\]
The basis for development of these stability conditions can be found in detail in a paper written by O'Brien, Hyman and Kaplan [8].

This procedure has a very important calculational advantage because there is no matrix inversion required.

**Purely Implicit Procedure**

By writing equation (1-2) at the \( n+1 \) level and then applying it and equation (1-3) to the general equation (1-1), one obtains the following implicit relationship:

\[
\varphi_{i,j,n} = \frac{\Delta T}{D_{i,j,n}} \left( \frac{D_n \varphi_{n+1}}{\Delta T} \right)_{i,j} - \left[ \Delta_x^2 \varphi_{i+1,j,n+1} + \Delta_y^2 \varphi_{i,j,n+1} + C_{i,j} \right]
\]

By writing equation (1-9) together with the appropriate initial and boundary conditions (1-5) and (1-6) for all points \( i,j \), one obtains a system of \( (N \times M) \) equations in \( (N \times M) \) unknowns. The solution of the system of equations can be expressed in matrix notation as:

\[
\tilde{X} = L^{-1} \tilde{K}
\]

where:

- \( \tilde{X} \) is a vector containing the values of \( \varphi_{i,j,n+1} \),
- \( L^{-1} \) is the inverse of the square coefficient matrix of order \( (N \times M) \),
\( \vec{K} \) is a vector containing the values of \( \left( \frac{\Delta T C_{i,j}}{D_{i,j,n}} \phi_{i,j,n+1} \right) \).

A difficulty in this technique develops because the coefficient \( A \) and \( B \) in (1-9) are functions of \( \phi_{i,j,n+1} \). This makes the system of equations nonlinear in the coefficients. One way to handle this is to let \( A \) and \( B \) lag one \( \Delta T \) increment, thus defining a quasi-linear system.

In some cases, \( A \) and \( B \) become in a sense iteration parameters, in which case the matrix \( L \) is constantly updated using the latest values of \( \phi_{i,j,n+1} \). This process continues until convergence occurs, i.e., until the \( \phi \)'s used to compute \( A \) and \( B \) and the ones computed are equal.

The purely implicit scheme is useful in the sense that it is stable for all \( \Delta T \) increments; however, a stable system is not necessarily convergent. Also the inversion of the large matrices, that result from this scheme, can be quite difficult and time consuming.

**Alternating-Direction Implicit**

By applying equation (1-2) written at the \( n+1 \) level to one of the second derivatives in equation (1-1), say \( \frac{\partial}{\partial x} \left[ A \frac{\partial \phi}{\partial x} \right] \),
and applying equation (I-2) written at the n level to the other derivative, \[ \frac{\partial}{\partial y} \left[ B \frac{\partial \phi}{\partial y} \right] \], one obtains:

\[ \Delta_x^2 (A\phi)_{i,j,n+1} + \Delta_y^2 (B\phi)_{i,n+1} + C_{i,j} = \left[ D_n \left( \frac{\phi_{n+1} - \phi_n}{\Delta T} \right) \right]_{i,j} \quad (I-11) \]

By writing (I-11) together with (I-5) and (I-6) at all points i for a particular j, one obtains a system of N equations in N unknowns implicit in the x direction. By repeating this for each j, one obtains M systems of equations which are solved for the unknowns, \( \phi_{i,j,n+1} \), where n is fixed.

Next the procedure is repeated for an equal \( \Delta T \) increment but this time the difference equations (I-12) are implicit in the y direction.

\[ \Delta_x^2 (A\phi)_{i,j,n+1} + \Delta_y^2 (B\phi)_{j,n+2} + C_{i,j} = \left[ D_n \left( \frac{\phi_{n+2} - \phi_{n+1}}{\Delta T} \right) \right]_{i,j} \quad (I-12) \]

Equation (I-12) together with (I-5) and (I-6) is written at all points j for a particular i, thus forming a system of M equations in M unknowns implicit in the y direction. By repeating this for each i, N systems of equations are formed which are then solved for the unknowns \( \phi_{i,j,n+2} \), where n is fixed.

Again a difficulty in this technique develops because the coefficient \( A \) in (I-11) is a function of \( \phi_{n+1} \) and the coefficient
B in (I-12) is a function of $\phi_{n+2}$. This condition makes the systems of equations nonlinear in the coefficients. This is handled by several different iteration schemes, some of which are discussed in [2,3,4].

**Newton's Technique**

Dempsey [1] proposed yet another technique for solving equation (I-1) numerically. It involves considering (I-1) at each $i,j$ as a set $F$ of $N \times M$ nonlinear equations over the reals where:

\[
F = \left\{ f_r \left| f_r(\phi_{1,1}, n+1, \phi_{1,2}, n+1, \ldots, \phi_{i,j}, n+1, \ldots, \phi_{N,M}, n+1) = 0 \right. \right\}
\]

for $r = 1, 2, \ldots, N \times M$, \hspace{1cm} (I-13)

or more concisely

\[
F = \left\{ \bar{f} \left| \bar{f}(\bar{\phi}) = 0 \right. \right\},
\]

where $\bar{\phi}$ is a vector containing the unknowns, $\phi_{n+1}$ and $\bar{f}$ is the column vector of functions $f_r$. If $\bar{\phi}_k$ is the $k$th approximation to the solution of (I-14) and $\bar{f}_k$ is written for $f(\bar{\phi}_k)$, then Newton's method [3,6] is defined by

\[
\bar{x}_{k+1} = \bar{x}_k - A_k^{-1} \bar{f}_k
\]

where $A_k$ is the Jacobian matrix $\frac{\partial f_r}{\partial x_p}$ evaluated at $x_k$. This pro-
procedure is quite useful since it lends itself quite readily to convergence analysis and allows for the consideration of completely nonlinear coefficients.

A detailed development of the mathematics involved in applying Newton's procedure to the nonlinear partial differential equation (1-1) is discussed in detail in Chapter II. The results of a sample problem and a rate of convergence study are presented in Chapter III and the conclusions and suggestions for future work in this area are presented in Chapter IV.
CHAPTER II

MATHEMATICAL DEVELOPMENT

In this chapter, a detailed discussion about Newton's technique for several variables (method of iteration, convergence, etc.) as discussed in [3,11,12] is presented. A detailed development of the technique as it applies to equation (I-1) together with its initial and boundary conditions (I-5) and (I-4) is also presented (see Dempsey [3]).

Determination of Grid System

Let \( P \) be the space \([0,G] \times [0,H]\) and let the domain of equation (I-1) be \( P \times [0,\infty) \). Proceeding, let

\[
S_1 = \{ x \in \mathbb{R} \mid x \in [0,G] \}, \quad (II-1)
\]

\[
S_2 = \{ y \in \mathbb{R} \mid y \in [0,H] \}, \quad (II-2)
\]

\[
S_3 = \{ t \in \mathbb{R} \mid t \in [0,\infty) \}. \quad (II-3)
\]

A grid \( K \) over \( P \) is determined by subdividing the interval \([0,G]\) into \( N+1 \) subintervals, the interval \([0,H]\) into \( M+1 \) subintervals and letting

\[
x = \sum_{k=1}^{1} \Delta x_k, \quad \text{where } i=0,1,2,\ldots,N+1,
\]
\[
    y = \sum_{k=1}^{j} \Delta y_k, \quad \text{where } j=0,1,2,\ldots,M+1,
\]

also the interval \([0,\infty)\) is subdivided with

\[
    t = \sum_{k=1}^{n} \Delta T_k, \quad \text{where } n=0,1,\ldots.
\]

**Formulation of Problem**

In expanding Newton's technique to \((N \times M)\) variables, one writes equation (I—1) together with its boundary conditions in appropriate difference form for all points \(i,j\) of the grid \(K\) and forms the set \(F\) of equations with continuous derivatives of all orders where:

\[
    F = \left\{ f_{i,j} \right\}
\]

\[
    f_{i,j} \left( [0,\ldots,\varphi_i,j-1,\varphi_i-1,j,\varphi_i,j,\varphi_i+1,j,\varphi_i,j+1,0,\ldots,0]_{n+1} \right) =
\]

\[
    \Delta^2_x \left( A\varphi \right)_{i,j,n+1} + \Delta^2_y \left( B\varphi \right)_{i,j,n+1} + C_{i,j} - \left[ \frac{(D\varphi)_{n+1} - (D\varphi)_n}{\Delta T} \right]_{i,j}
\]

where \(i=1,2,\ldots,N; j=1,2,\ldots,M\) \hspace{1cm} (II—4)

The expansion of a particular \(f_{i,j}\) into a Taylor series gives the following equation:
\[ f_{i+1,j} ([0, \ldots, \psi_{i+1,j-1}, \psi_{i+1,j}, \psi_{i+1,j-1}, \psi_{i+1,j}, \psi_{i+1,j}+1, \psi_{i+1,j+1}, 0, \ldots, 0]_{n+1}) = \]
\[
\begin{pmatrix}
\psi_{i+1,j} ([0, \ldots, \varphi_{i+1,j-1}, \varphi_{i+1,j}, \varphi_{i+1,j-1}, \varphi_{i+1,j}, \varphi_{i+1,j}+1, \varphi_{i+1,j+1}, 0, \ldots, 0]_{n+1}) + \\
\left[
\begin{array}{c}
\frac{\partial f_{i,j}}{\partial \varphi_{i,j-1}}, j \frac{\partial f_{i,j}}{\partial \varphi_{i,j-1}}, j + \frac{\partial f_{i,j}}{\partial \varphi_{i,j}}, j + \frac{\partial f_{i,j}}{\partial \varphi_{i,j+1}}, j + \frac{\partial f_{i,j}}{\partial \varphi_{i,j+1}}, j \\
\frac{\partial \varphi_{i,j}}{\partial \varphi_{i,j-1}}, j + \frac{\partial \varphi_{i,j-1}, j}{\partial \varphi_{i,j}} + \frac{\partial \varphi_{i,j+1}, j}{\partial \varphi_{i,j}}, j + \frac{\partial \varphi_{i,j+1}, j}{\partial \varphi_{i,j+1}, j}
\end{array}
\right]
\end{pmatrix}^{n+1} + \text{higher order terms,} \tag{II-5}
\]

where:
\[ \psi_n = \varphi + \Delta \varphi. \]

Let us now make the following definitions:

\[ \frac{\partial f_{i,j}}{\partial \varphi_{i,j-1}, j} = D_{i+1,j} \tag{II-6} \]

\[ \frac{\partial f_{i,j}}{\partial \varphi_{i,j-1}, j, n+1} = D_{i+1,j} \tag{II-7} \]

\[ \frac{\partial f_{i,j}}{\partial \varphi_{i,j+1}, j} = D_{i+1,j} \tag{II-8} \]

\[ \frac{\partial f_{i,j}}{\partial \varphi_{i,j+1}, j, n+1} = D_{i+1,j} \tag{II-9} \]
\[
\frac{\partial f_{1,j}}{\partial \phi_{1,j+1,n+1}} = D_{5,1,j}.
\] (II-10)

By writing (II-5) at all points \(i,j\) of \(K\), truncating at the first order terms and setting the right side equal to zero, one obtains a set of \((N \times M)\) simultaneous equations which are now linear in the unknowns, the \(\Delta \phi\)'s.

One obtains the following upon rearrangement of the terms:

\[
D_{1,i,j} \Delta \phi_{i,j-1} + D_{2,i,j} \Delta \phi_{i-1,j} + D_{3,i,j} \Delta \phi_{i,j} + D_{4,i,j} \Delta \phi_{i+1,j} +
\]

\[
D_{5,i,j} \Delta \phi_{i,j+1} = -f_{1,j} ([0, \ldots, \phi_{i,j-1}', \phi_{i-1,j}', \phi_{i,j}', \phi_{i,j+1}', 0]_{n+1}^\top).
\] (II-11)

Figure 1 gives a matrix representation of a special case of the above system of equations.

The coefficient \(D_{3,i,j}\) (see equation (II-8)) will be expanded in detail to illustrate the method of handling the approximations for the other coefficients.

\[
D_{3,i,j} = \frac{\partial f_{1,j}}{\partial \phi_{1,j,n+1}} =
\]
The coefficients \( D_1, D_2, \ldots, D_5 \) are initially approximated with \( \phi_{i,j,n+1} = \phi_{i,j,n} \). The resulting system of equations is then solved for the \( \Delta \phi_{i,j}'s \). The values of the \( \Delta \phi_{i,j}'s \) are checked against zero or some acceptable tolerance. If the tolerance condition is not met, let

\[
\phi_{i,j,n+1} = \phi_{i,j,n+1} + \Delta \phi_{i,j},
\]

evaluate the coefficients again and repeat the iteration process.

(See next two sections for step by step explanation of iteration process and derivation of sufficient conditions for convergence.)

**Method of Iterative Solution**

A brief description of the process advanced by Dempsey [3] to solve equation (I-1) is now illustrated using two-dimensional
functions.

(1) Let \( f^1(01,02) = 0 \) and \( f^2(01,02) = 0 \) where \( f^1 \) and \( f^2 \) are nonlinear functions of \( 01 \) and \( 02 \) with continuous derivatives of the second order. Also, let \((01_s,02_s)\) be the solution.

(2) Expand \( f^1 \) and \( f^2 \) into a Taylor's series of two variables in which the \( \Delta \)'s are the linear deviations from the zeroes of \( f^1 \) and \( f^2 \).

\[
f^1(01 + \Delta 01, 02 + \Delta 02) = f^1(01, 02) + \Delta 01 f^1_{01}(01, 02) + \Delta 02 f^1_{02}(01, 02) + \ldots \]

\[
f^2(01 + \Delta 01, 02 + \Delta 02) = f^2(01, 02) + \Delta 01 f^2_{01}(01, 02) + \Delta 02 f^2_{02}(01, 02) + \ldots .
\]

(3) Truncate the series at the first order terms. Set the right hand side equal to zero, thus the two equations remaining are now linear in \( \Delta 01 \) and \( \Delta 02 \).

(4) Let \( 01_1 = 01_s \) and \( 02_1 = 02_s \). Evaluate \( f^1, f^2, f^1_{01}, f^2_{01}, f^1_{02}, \) and \( f^2_{02} \) at \((01_1, 02_1)\).
(5) After substituting these values into the truncated right hand side, solve for $\Delta \phi_1$ and $\Delta \phi_2$.

(6) Check the values of $\Delta \phi_1$ and $\Delta \phi_2$ against zero or some other acceptable tolerance.

(7) If the values of $\Delta \phi_1$ and $\Delta \phi_2$ have met an acceptable tolerance, then the current values of $(\phi_1, \phi_2)$ are the zeroes of $f^1$ and $f^2$ or a very close approximation to them.

(8) If the tolerance condition is not met, let $\phi_1^s \equiv \phi_1^1 + \Delta \phi_1$ and $\phi_2^s \equiv \phi_2^1 + \Delta \phi_2$ and evaluate the functions and their partial derivatives again and then repeat the process from step 5.

Convergence of the Iterative Process

The sufficient conditions for convergence of this technique are now found for a function of two variables. This convergence analysis can readily be extended to $n$ variables.

Given the two equations,

$$ f(\phi_1, \phi_2) = 0, \quad (\text{II-13}) $$

$$ g(\phi_1, \phi_2) = 0, \quad (\text{II-14}) $$

write them in the form
\[ \phi_1 = F_1(\phi_1, \phi_2) = \phi_1 - \left( \frac{\partial g}{\partial \phi_2} - g \frac{\partial f}{\partial \phi_2} \right) \frac{\partial f}{\partial \phi_1} \frac{\partial g}{\partial \phi_1} - \frac{\partial f}{\partial \phi_2} - \frac{\partial f}{\partial \phi_1} \frac{\partial g}{\partial \phi_1} \right), \quad (II-15) \]

\[ \phi_2 = F_2(\phi_1, \phi_2) = \phi_2 + \left( \frac{\partial g}{\partial \phi_1} - g \frac{\partial f}{\partial \phi_1} \right) \frac{\partial f}{\partial \phi_2} \frac{\partial g}{\partial \phi_2} - \frac{\partial f}{\partial \phi_2} - \frac{\partial f}{\partial \phi_1} \frac{\partial g}{\partial \phi_1} \right) \phi_1, \phi_2 \quad (II-16) \]

These equations are satisfied by the exact values of the zeroes \( \phi_{1s}, \phi_{2s} \). Let \( \phi_{1o}, \phi_{2o} \) be approximate values of the zeroes. Improved values are found by the following equations:

\[ \phi_{1o} = F_1(\phi_{1o}, \phi_{2o}), \quad (II-17) \]

\[ \phi_{2o} = F_2(\phi_{1o}, \phi_{2o}). \quad (II-18) \]

Subtracting these two equations from the corresponding ones above, one obtains:

\[ \phi_1 - \phi_{1o} = F_1(\phi_1, \phi_2) - F_1(\phi_{1o}, \phi_{2o}), \quad (II-19) \]

\[ \phi_2 - \phi_{2o} = F_2(\phi_1, \phi_2) - F_2(\phi_{1o}, \phi_{2o}). \quad (II-20) \]

Let

\[ \phi_1 \approx \phi_{1o} + \Delta \phi_{1o}, \quad (II-21) \]
\[ \varphi_2 \equiv \varphi_2^o + \Delta \varphi_2^o, \quad (II-22) \]

and expand \( F_1 \) and \( F_2 \) into a Taylor's series with all terms higher than first order truncated. Thus,

\[ F_1(\varphi_1^o + \Delta \varphi_1^o, \varphi_2^o + \Delta \varphi_2^o) - F_1(\varphi_1^o, \varphi_2^o) \equiv \Delta \varphi_1^o \frac{\partial F_1}{\partial \varphi_1} + \Delta \varphi_2^o \frac{\partial F_1}{\partial \varphi_2}, \quad (II-23) \]

\[ F_2(\varphi_1^o + \Delta \varphi_1^o, \varphi_2^o + \Delta \varphi_2^o) - F_2(\varphi_1^o, \varphi_2^o) \equiv \Delta \varphi_1^o \frac{\partial F_2}{\partial \varphi_1} + \Delta \varphi_2^o \frac{\partial F_2}{\partial \varphi_2}. \quad (II-24) \]

Substituting into (II-19) and (II-20), one obtains

\[ \varphi_1 - \varphi_1^o = \Delta \varphi_1^o \frac{\partial F_1}{\partial \varphi_1} + \Delta \varphi_2^o \frac{\partial F_1}{\partial \varphi_2}, \quad (II-25) \]

and

\[ \varphi_2 - \varphi_2^o = \Delta \varphi_1^o \frac{\partial F_2}{\partial \varphi_1} + \Delta \varphi_2^o \frac{\partial F_2}{\partial \varphi_2}. \quad (II-26) \]

Applying the triangle inequality to (II-25) and (II-26) and then adding the two equations, one obtains:

\[ |\varphi_1 - \varphi_1^o| + |\varphi_2 - \varphi_2^o| \leq \Delta \varphi_1^o \left( \left| \frac{\partial F_1}{\partial \varphi_1} \right| + \left| \frac{\partial F_2}{\partial \varphi_1} \right| \right) \]

\[ + \Delta \varphi_2^o \left( \left| \frac{\partial F_1}{\partial \varphi_2} \right| + \left| \frac{\partial F_2}{\partial \varphi_2} \right| \right). \quad (II-27) \]

Choose a value \( \Phi \) such that
\[
\left( \left| \frac{\partial F}{\partial \phi_1} \right| + \left| \frac{\partial F}{\partial \phi_2} \right| \right) \leq P \quad \text{and} \quad \left( \left| \frac{\partial F}{\partial \phi_1} \right| + \left| \frac{\partial F}{\partial \phi_2} \right| \right) \leq P \quad (11-28)
\]

for all points in the region \((\phi_1, \phi)\) and \((\phi_2, \phi)\).

Then (11-27) becomes

\[
\left| \phi_1 - \phi_1 \right| - \left| \phi_2 - \phi_2 \right| \leq P \left( \left| \Delta \phi_1 \right| + \left| \Delta \phi_2 \right| \right),
\]

or, using equations (11-21) and (11-22),

\[
\left| \phi_1 - \phi_1 \right| - \left| \phi_2 - \phi_2 \right| \leq P \left( \left| \phi_1 - \phi_1 \right| + \left| \phi_2 - \phi_2 \right| \right). \quad (11-29)
\]

Relation (11-29) holds for the first approximation. Similar relations result for subsequent approximations, thus one obtains:

\[
\left| \phi_1 - \phi_1 \right| + \left| \phi_2 - \phi_2 \right| \leq P \left( \left| \phi_1 - \phi_1 \right| + \left| \phi_2 - \phi_2 \right| \right)
\]

\[
\left| \phi_1 - \phi_n \right| + \left| \phi_2 - \phi_n \right| \leq P \left( \left| \phi_1 - \phi_n \right| + \left| \phi_2 - \phi_n \right| \right)
\]

By repeated substitution one obtains:

\[
\left| \phi_1 - \phi_n \right| + \left| \phi_2 - \phi_n \right| < P^n \left( \left| \phi_1 - \phi_1 \right| + \left| \phi_2 - \phi_2 \right| \right). \quad (11-30)
\]

From relation (11-30) one sees that the quantities \( \left| \phi_1 - \phi_n \right| \) and \( \left| \phi_2 - \phi_n \right| \) can be made as small as one wants if there exists a P
less than 1 satisfying equation (II-28).

Thus, Newton's iteration process converges when

\[ \left| \frac{\partial F_1}{\partial \varphi_1} \right| + \left| \frac{\partial F_2}{\partial \varphi_2} \right| < 1 \]

and

\[ \left| \frac{\partial F_1}{\partial \varphi_2} \right| + \left| \frac{\partial F_2}{\partial \varphi_2} \right| < 1 \]

throughout the domain of \((\varphi_1, \varphi_2)\).
Matrix Entries with N = 3, M = 3 Using Outlined Procedure

SAMPLE MATRIX ENTRIES

FIGURE 1
CHAPTER III

RESULTS

In this chapter, the solution of equation (I-1) together with its initial and boundary conditions with Newton's iterative technique is compared with a modified alternating direction iterative technique (see Dempsey [3]). In addition, the rate of convergence of Newton's iterative technique (as applicable to the specific equation being studied) is investigated in detail (see Kunz [7]).

Sample Problem

In order to compare Newton's iterative technique (hereafter referred to as Model 1) with the modified alternating direction technique (hereafter referred to as Model 2), the following sample problem was solved.

Using the notation found at the beginning of Chapter II, let

\[ s_1 = \{ x \in \mathbb{R} \mid x \in [0, 0.6336] \} \]

and

\[ s_2 = \{ y \in \mathbb{R} \mid y \in [0, 0.6336] \} \] .

The interval [0, 0.6336] is divided into 12 equal subintervals;
thus

\[ \Delta x_k = \Delta y_L = 528 \] where \( k = 1, 2, \ldots, 12 \)

\[ L = 1, 2, \ldots, 12 \] .

Also,

\[ s_3 = \left\{ t \in \mathbb{R} \mid t \in [0, 15] \right\} \] with \( \Delta T = 1 \) .

Proceeding, let

\[ \overline{\phi}(x, y, t) = 2 \phi(x, y, t) - \frac{\phi(x, y, t)_{\text{max}} + \phi(x, y, t)_{\text{min}}}{\phi(x, y, t)_{\text{max}} - \phi(x, y, t)_{\text{min}}} \] ,

where \( \phi(x, y, t)_{\text{max}} \) and \( \phi(x, y, t)_{\text{min}} \) are prescribed maximum and minimum values of \( \phi(x, y, t) \) with \( \phi(x, y, t)_{\text{max}} = 3500 \), and

\( \phi(x, y, t)_{\text{min}} = 500 \);

\[ A(\phi(x, y, t), x, y) = B(\phi(x, y, t), x, y) = 50 \left( 1.4 \times 10^5 + 7.0 \times 10^4 \overline{\phi}(x, y, t) - 2.9 \times 10^4 \overline{\phi}(x, y, t)^2 \right) ; \]

\[ D(\phi(x, y, t), x, y) = \frac{592.5}{(0.88 - 0.03 \phi(x, y, t) + 0.05 \overline{\phi}(x, y, t)^2) \right) , \]

where the polynomials which are used to approximate the coefficients \( A, B \) and \( D \) were calculated by a regression technique;
The initial condition for this problem is \( \varphi(x, y, 0) = 3300 \).

Figure 2 compares the solutions obtained by Model 1 and Model 2 graphically. The slight difference in the two solutions can be attributed to two things:

1. **Difference in closure criteria** -
   
   In Model 1, the specification for convergence is that
   \[
   \Delta \varphi_{i,j,n+1} < 1 \times 10^{-4} \text{ for all } i,j \text{ and a particular } n.
   \]
   
   In Model 2, the specification for convergence is that
   \[
   \frac{\Delta \varphi_{i,j,n+1}}{\sum_{ij} \Delta \varphi_{i,j,n+1}} < 1 \times 10^{-5} \text{ for all } i,j \text{ and a particular } n.
   \]

2. **Different ways of handling the coefficients A, B and D** -
   
   In Model 1, the coefficients A, B and D are updated with every iteration; thus the entire coefficient matrix is updated.

   In Model 2, the coefficients A, B and D are evaluated by using values of \( \varphi_{i,j,n} \). The main diagonal of the coefficient matrix is updated with every iteration by use of an iteration parameter.
\[ \Phi_{6,6} \]

CUMULATIVE T

COMPARISON RUN FOR SAMPLE DATA

FIGURE 2
Figures 3, 4 and 5 compare the convergence of $\Delta \phi_{6,6,1}$. The $\Delta T$ values used in calculating the values for the 3 graphs were 1, 2 and 4 respectively.

It should be noted that Model 1 and Model 2 are basically the same in this particular instance on the first iteration. For the second and third iterations, Model 1 always approaches zero from the positive side and Model 2 always approaches zero from the negative side. In the author's opinion, this difference is caused because the coefficients A, B and D are handled differently in Model 1 and Model 2. By appropriate choice of the iteration parameter the convergence graph of Model 2 would very closely approximate that of Model 1.
CONVERGENCE COMPARISON

RUN 1
MODEL 1
MODEL 2
T = 1

FIGURE 3
\[ \Delta \phi_{6,6} \]

**CONVERGENCE COMPARISON 2**

**FIGURE 4**

RUN 2
MODEL 1
MODEL 2
T = 2
CONVERGENCE COMPARISON 3

RUN 3
MODEL 1
MODEL 2
T = 4

ITERATION #

FIGURE 5
Rate of Convergence

The rate of convergence was studied by the following technique. Consider the following function $F$:

Let

$$F = f(0, \ldots, (\phi_s)_{i,j-1,n+1}, (\phi_s)_{i-1,j,n+1}, \phi_{i,j,n_k},$$

$$(\phi_s)_{i+1,j,n+1}, (\phi_s)_{i,j+1,n+1}, 0, \ldots, 0)$$

where the $(\phi_s)$'s are the actual roots of $F$ to the accuracy required and $\phi_{i,j,n_k}$ is an approximate value of

$$(\phi_s)_{i,j,n+1}$$

at the $k$th iteration.

Observing that $F$ is a function of $\phi_{i,j,n_k}$ only, let us call this function $G(\phi_{i,j,n_k})$.

Proceeding, find some $P$ such that

$$\left| \frac{G''(\xi)}{2G'(\phi_{i,j,n_k})} \right| < P$$

where $\phi_{i,j,n_k} < \xi < (\phi_s)_{i,j,n+1}$.

$\phi_{i,j,n_k}$ is said to approximate $(\phi_s)_{i,j,n+1}$ to $p$ decimal places where $p$ is the greatest integer less than $-\log \left| \phi_{i,j,n_k} \right|$.
Having determined $p$, one can predict the decimal place accuracy of $\phi_{i,j,n}^{s_{i,j,n+1}}$ by the following relationship:

$$\phi_{i,j,n}^{s_{i,j,n+1}} \text{ approximates } (\phi_{i,j,n+1}^{s_{i,j,n+1}}) \text{ to } r \text{ decimal places}$$

where $r$ is the greatest integer less than $2p - \log P$.

By using this technique on all points $\phi_{i,j,n+1}^{s_{i,j,n+1}}$ for a fixed $n+1$, one can predict the "after the fact" convergence of all the $\phi$'s on the grid $K$. With enough of this "after the fact" convergence history, one could hopefully be able to develop some parameter dependent analytical expressions, $\psi$(prediction parameter), which could be used in addition to the $\Delta$'s to predict the a priori convergence of a particular problem.
CHAPTER IV

CONCLUSIONS AND RECOMMENDATIONS

The work described here is an investigation of Newton's technique for several variables as applied to multi-dimensional nonlinear problems. A computer program was written which applied the technique to the nonlinear partial differential equation presented in Chapter I. The results obtained have shown that Newton's technique for several variables is general enough to be applied successfully to multi-dimensional nonlinear problems. The technique is convergent for at least a practical range of variables and within this range has an extremely rapid rate of convergence.

The results obtained from the technique compare quite favorably with other accepted techniques for solving multi-dimensional nonlinear problems as was briefly illustrated in Chapter III with a sample problem.

One of the principal advantages of Newton's technique is that it enables one to measure the "after the fact" convergence of the unknowns. This "measuring" process can be accomplished by using the rate of convergence technique described in Chapter III. By use of this technique one is able to predict for the following iteration the nearness (in terms of significant figures) of the actual
roots to the calculated roots. By use of "after the fact" convergence histories, one can develop analytical expressions to predict convergence "before the fact," thus enabling an even faster rate of convergence.

The author recommends that future work on this topic be done in the three following areas:

(1) The actual development of parameter dependent analytical expressions to be used in predicting "before the fact" convergence. The author suggests correlation analysis as a possible starting point in this development.

(2) An investigation into possible modifications of Newton's technique to permit less frequent updating of the Jacobian matrix without drastically affecting the rate of convergence. As presented, the Jacobian matrix must be updated on every iteration.

(3) The application of Newton's technique to the three dimensional form of Equation (1-1).
BIBLIOGRAPHY


