



A new iterative method for solving simultaneous linear equations with direct applications to three-dimensional heat conduction problems
by Rodney Paul Horning

A thesis submitted in partial fulfillment of the requirements for the degree of MASTER OF SCIENCE
in Mechanical Engineering
Montana State University
© Copyright by Rodney Paul Horning (1980)

Abstract:

A recently developed iteration method for solving simultaneous linear equations is considered. Previously, rapid convergence of the algorithm was not guaranteed due to unestablished criteria for trial solution generation. A systematic trial solution generation routine is introduced and the new method is used to solve three-dimensional heat conduction problems. Examples of a steady state problem and a transient problem each with 1000 unknowns demonstrate the new method's performance as compared to existing techniques. Results indicate that the new method is superior for the transient case.

STATEMENT OF PERMISSION TO COPY

In presenting this thesis in partial fulfillment of the requirements for an advanced degree at Montana State University, I agree that the Library shall make it freely available for inspection. I further agree that permission for extensive copying of this thesis for scholarly purposes may be granted by my major professor, or, in his absence, by the Director of Libraries. It is understood that any copying or publication of this thesis for financial gain shall not be allowed without my written permission.

Signature Rodney Paul Henning
Date August 28, 1980

A NEW ITERATIVE METHOD FOR SOLVING SIMULTANEOUS LINEAR
EQUATIONS WITH DIRECT APPLICATIONS TO THREE-
DIMENSIONAL HEAT CONDUCTION PROBLEMS

by

RODNEY PAUL HORNING

A thesis submitted in partial fulfillment
of the requirements for the degree

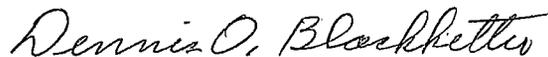
of

MASTER OF SCIENCE

in

Mechanical Engineering

Approved:


Chairperson, Graduate Committee


Head, Major Department


Graduate Dean

MONTANA STATE UNIVERSITY
Bozeman, Montana

August, 1980

ACKNOWLEDGMENTS

The author wishes to thank Dr. D. O. Blacketter and Dr. R. O. Warrington for their help and guidance in the performance of this study.

TABLE OF CONTENTS

	<u>Page</u>
VITA	ii
ACKNOWLEDGMENTS	iii
LIST OF TABLES	v
LIST OF FIGURES	vi
NOMENCLATURE	vii
ABSTRACT	x
CHAPTER I. INTRODUCTION	1
CHAPTER II. DESCRIPTION OF METHOD	4
CHAPTER III. GENERATION OF TRIAL SOLUTIONS	9
CHAPTER IV. APPLICATION AND RESULTS	21
CHAPTER V. CONCLUSION	41
LITERATURE CITED	43
APPENDICES:	
A. EXAMPLE OF THE NEW METHOD SHOWING CONSEQUENCES OF DIFFERENT TRIAL SOLUTION SELECTION	45
B. SOLUTION OF EQUATIONS (3.25 - 3.27) AND RESULTS OF EACH ITERATION	50

LIST OF TABLES

<u>Table</u>		<u>Page</u>
4.1	Cube-Cube Results for Various Values of m	26
4.2	Cube-Cube Results for Various SOR Factors	28
4.3	Summary of Transient Problem Results for New Method	32
4.4	Summary of Transient Problem Results for ADEP	34

LIST OF FIGURES

<u>Figure</u>		<u>Page</u>
3.1	Nodal Grid for Equation (3.22)	17
4.1	Cube-Cube Orientation	23
4.2	Execution Time of Different Numbers of Trial Solutions and Different Relaxation Factors	29
4.3	ADEP versus New Method at $\tau=0.1$	35
4.4	ADEP versus New Method at $\tau=0.5$	36
4.5	ADEP versus New Method at $\tau=1.0$	37
4.6	Computer Flowchart For New Method	40

NOMENCLATURE

<u>Symbol</u>	<u>Description</u>
A	heat generation (non-dimensional) (Equation 3.24)
c	unknown constant that relates the resulting temperature node due to heat generation at that node (Equation 3.12)
D	limiting effect distance (Equation 3.12)
d	nodal distance (Equation 3.12)
$\{e_i\}$	error matrix or residual of the approximate solution of iteration level i (Equation 2.4)
$\bar{e}_{i,j}$	specific coefficient of $\{e_i\}$ at matrix position i (Equation 3.12)
$\{e'\}$	desired average error matrix that signifies solution is reached (Equation 2.7)
\bar{e}'	the desired average error (Equation 2.7)
e''''	errors viewed as heat generation (Equation 3.10)
$\{F\}$	right hand matrix (Equation 2.2)
\bar{F}_j	specific coefficient of $\{F\}$ at matrix position j (Equation 2.1)
$[K]$	general coefficient matrix (Equation 2.2)
$\bar{K}_{j,k}$	specific coefficient of $[K]$ at matrix position j,k (Equation 2.1)
m	number of trial solutions (Equation 2.3)
n	number of unknowns (Equation 2.1)
q'	heat flux of concentric spheres (Equation 4.4)
r_i	inside sphere radius (Equation 4.4)

<u>Symbol</u>	<u>Description</u>
r_0	outside sphere radius (Equation 4.4)
r_1	coordinate in three dimensions corresponding to a nodal spacing of one
r_2	coordinate in three dimensions corresponding to a nodal spacing of $\sqrt{2}$
r_3	coordinate in three dimensions corresponding to a nodal spacing of $\sqrt{3}$
T	variable for temperature (Equation 4.1)
V	desired variance of solution (Equation 2.7)
V_i	variance associated with the approximate solution of iteration level i (Equation 2.5)
$\{X\}$	general matrix of unknowns (Equation 2.2)
\bar{X}_j	specific unknown of $\{X\}$ at matrix position j (Equation 2.1)
X	variable (Equation 3.22)
$\{X_i\}$	approximation of $\{X\}$ at iteration level i (Equation 2.3)
$[x_{i,j}]$	matrix number j used in the linear combination of approximate solution $\{X_i\}$ (Equation 2.3)
$\{x_i^!\}$	correction matrix added to $\{X_i\}$ (Equation 3.6)
$\bar{x}_{i,j}^!$	specific coefficient of $\{x_i^!\}$ at matrix position j (Equation 3.9)
x'	variable (Equation 3.10)
x	spacial coordinate (Equation 4.1)
y	spacial coordinate (Equation 4.1)
z	spacial coordinate (Equation 4.1)

<u>Symbol</u>	<u>Description</u>
$\alpha_{i,j}$	weighting coefficient for trial solution number j of iteration level i (Equation 2.3)
Δx	nodal spacing of finite difference approximation
Δy	nodal spacing of finite difference approximation
Δz	nodal spacing of finite difference approximation
θ	function of distance that describes the shape of the temperature profile (Equation 3.12)
π	constant 3.14159 (Equation 4.4)
τ	elapsed time (non-dimensional) (Equation 4.5)

Subscripts

e	corresponding to the error matrix (Equation 3.18)
i	iteration level (Equation 2.3)
j	matrix position (Equation 2.3)
k	variable (Equation 2.2)
D	corresponding to the limiting effect distance (Equation 3.19)
LB	corresponding to the last best solution (Equation 3.21)

Superscripts

t	transpose of matrix (Equation 2.5)
-----	------------------------------------

ABSTRACT

A recently developed iteration method for solving simultaneous linear equations is considered. Previously, rapid convergence of the algorithm was not guaranteed due to unestablished criteria for trial solution generation. A systematic trial solution generation routine is introduced and the new method is used to solve three-dimensional heat conduction problems. Examples of a steady state problem and a transient problem each with 1000 unknowns demonstrate the new method's performance as compared to existing techniques. Results indicate that the new method is superior for the transient case.

CHAPTER I
INTRODUCTION

Ever increasing demands by engineers for better accuracy from numerical methods that solve large systems of simultaneous equations has produced many excellent algorithms. A new iterative technique is presented here that has definite possibilities of joining the ranks of these highly regarded methods.

The new method [1] uses a linear combination of trial solutions with each trial solution having an unknown scalar weighting coefficient. Each weighting coefficient is solved for by minimizing an error function of the coefficients. The minimizing process generates a much smaller set of simultaneous equations with the coefficients as the unknowns. Thus when solving a large system of linear equations, the new method reduces the number of equations so that it can be solved easily by direct methods.

This new method is remotely related to the conjugate direction method, or CD method [2,3], as both are error function minimization routines. The CD method minimizes the error along specific directions that are conjugate, or orthogonal, to each other and thus the name. The CD method converges to the solution in less steps than there are unknowns if round-off error is eliminated. The methods have been shown [1] to be different.

Because the squared residual which is a function of several unknowns is minimized in the new method it can be related to the method of least squares [4,5]. The least square method determines the equation of a curve passing through many scattered points such that the sum of the squared distances from each point to the curve is minimized. The new method uses a closely related technique that the sum of the squares of the residuals of an approximate solution is minimized. The use of the least squares technique is usually applied to curve fitting and not to solving sets of simultaneous equations.

To compare the performance of the new method, two existing techniques were used: the first was the SOR method [6] with a relaxation factor, and the second was the Alternating Direction Explicit Procedure [6]. Both methods are highly regarded numerical methods [6] and are excellent choices of comparison techniques because of their speed and accuracy [6,8].

The theory of the new method had been completed but a systematic procedure had not been perfected for selecting trial solutions for the set of equations being solved. Good trial solution selection is essential for rapid convergence of the method. Because of the dependence on the characteristics of the set of equations to be solved, it was necessary to focus on one class of equations to determine a trial solution generation scheme for that class.

It is the purpose of this paper to present a trial solution generation scheme to be used with the new method [1] that together produce rapid enough convergence to be competitive with existing methods.

CHAPTER II

DESCRIPTION OF METHOD

The new method is an iterative procedure. At the beginning of an iteration, an approximation of the solution to the set of equations is made that consists of a linear combination of several linearly independent solution vectors. Each vector is assigned an unknown weighting coefficient. The method solves for the weighting coefficients so that the error of the solution approximation is minimized. To do this, the linear combination of vectors with the unknown weighting coefficients are substituted into the set of equations being solved. The residuals of the approximation are squared and summed to create an error function whose variables are the weighting coefficients. This error function, or variance, is minimized by setting its partial derivatives with respect to the unknown coefficients equal to zero.

A new smaller set of simultaneous linear equations results, whose size is determined by the number of unknown coefficients. These equations can be solved for the values of the coefficients by a direct method that produces accurate results with very little or no round-off error.

By substituting the coefficients into the linear combination of the approximate solution, a better estimate of the solution is achieved. The next iteration begins with an unknown weighting coefficient assigned to the improved solution just generated and is used in the

linear combination along with other trial vectors in the next approximation. The method iterates on these steps until a solution is reached that has sufficient accuracy.

The following pages of this section will be concerned with the problem of solving the following nxn system of linear equations

$$\begin{aligned} \bar{K}_{1,1}\bar{X}_1 + \bar{K}_{1,2}\bar{X}_2 + \dots + \bar{K}_{1,n}\bar{X}_n &= \bar{F}_1 \\ \bar{K}_{2,1}\bar{X}_1 + \bar{K}_{2,2}\bar{X}_2 + \dots + \bar{K}_{2,n}\bar{X}_n &= \bar{F}_2 \\ \dots & \dots \dots \dots \dots \\ \bar{K}_{n,1}\bar{X}_1 + \bar{K}_{n,2}\bar{X}_2 + \dots + \bar{K}_{n,n}\bar{X}_n &= \bar{F}_n \end{aligned} \quad (2.1)$$

particularly where n is so large that it makes using direct methods inaccurate due to the accumulation of round-off errors (usually larger than 40 equations [6]). These equations will be written in the matrix form

$$[K]\{X\} = \{F\} \quad (2.2)$$

where [K] is the matrix of coefficients $\bar{K}_{j,k}$, $j=1,n$, $k=1,n$, and {X} and {F} are the vectors \bar{X}_j and \bar{F}_j , $j=1,n$, respectively.

An approximate solution, $\{X_i\}$, to Equation (2.2) at iteration level i is a linear combination of m linearly independent trial solutions, $[x_{i,j}]$, $j=1,m$, with unknown scalar weighting coefficients

$\alpha_{i,j}$,

$$\{X_i\} = \sum_{j=1}^m \alpha_{i,j} [x_{i,j}]. \quad (2.3)$$

An expression for the error vector, $\{e_i\}$, of the approximate solution, $\{X_i\}$, is formed by the substitution of Equation (2.3) into Equation (2.2)

$$[K]\{X_i\} - \{F\} = \{e_i\} \quad (2.4)$$

and the squared residual, or variance, is

$$V_i(\alpha_{i,1}, \dots, \alpha_{i,m}) = \{e_i\}^t \{e_i\}. \quad (2.5)$$

In order to minimize V_i , Equation (2.5), with the appropriate values of the weighting coefficients, $\alpha_{i,1}, \dots, \alpha_{i,m}$, the partial derivatives of V_i with respect to each unknown weighting coefficient is set equal to zero

$$\frac{\partial V_i}{\partial \alpha_{i,j}} = 0, \quad j=1, m. \quad (2.6)$$

Thus for the original n unknowns in Equation (2.1) and m trial solutions in Equation (2.3), m unknown weighting coefficients with m equations result from Equation (2.6). A direct method can be used to solve the set of equations resulting from Equation (2.6), if the magnitude of m is not so large as to make the direct method inaccurate and overly time consuming [6].

By substituting the known weighting coefficients from solving the $m \times m$ system of Equation (2.6) into Equation (2.3), the approximation $\{X_i\}$ is known. As a measure of the goodness of $\{X_i\}$ as the solution to Equation (2.2), the known weighting coefficients are substituted into

Equation (2.5) to determine a numerical value of the variance. An approximation of V_i before an acceptable approximation of $\{X\}$ of Equation (2.2) is achieved can be made by summing the squares of the desired absolute average error, $\{e'\}$, or

$$V \leq n(\bar{e}')^2 \quad (2.7)$$

If the value of V_i does not satisfy the desired variance of Equation (2.7), iteration level $i+1$ is started by setting the first trial solution $[x_{i+1,1}]$ of Equation (2.3) equal to the approximate solution of the previous iteration level:

$$[x_{i+1,1}] = \{X_i\} \quad (2.8)$$

and by selecting the additional trial solutions

$$[x_{i+1,j}], j=2,m \quad (2.9)$$

the next approximation of $\{X\}$ in Equation (2.2) becomes

$$\{X_{i+1}\} = \sum_{j=1}^m \alpha_{i+1,j} [x_{i+1,j}]. \quad (2.10)$$

The preceding steps, Equations (2.4) through (2.6), are then repeated until an approximation of $\{X\}$ of Equation (2.2) is found that has a variance less than or equal to the desired variance approximated by Equation (2.7).

The approximation $\{X_i\}$ has associated with it the variance V_i . For iteration level $i+1$, $\{X_i\}$ becomes $[x_{i+1,1}]$ with the unknown weight-

ing coefficient $\alpha_{i+1,1}$. Consider the worst case that the other trial solutions, $[x_{i+1,j}]$, $j=2,m$, cannot improve the approximation $\{X_{i+1}\}$ no matter what values are assigned to their weighting coefficients, $\alpha_{i+1,j}$, $j=2,m$; therefore, their coefficients would be zero and $\alpha_{i+1,1}$ would be unity. Thus, $\{X_{i+1}\}$ would equal $\{X_i\}$ and both approximations would have associated with them the same variance V_i . But if any improvement could be made in the approximate solution $\{X_{i+1}\}$ the weighting coefficients, $\alpha_{i+1,j}$, $j=2,m$, would not all be zero and the improvement in the approximation of $\{X\}$ would result in a smaller variance V_{i+1} [6]. Therefore, the variance at level $i+1$ will always be less than or equal to the variance of the previous iteration

$$V_{i+1} \leq V_i \quad (2.11)$$

The proper selection of trial solutions $[x_{i+1,j}]$, $j=2,m$ is paramount to achieving rapid convergence using this new technique. Previous investigators [1] provide an excellent example that demonstrates the new method and the consequences of different trial solution selection and it is repeated in Appendix A.

CHAPTER III

GENERATION OF TRIAL SOLUTIONS

A general algorithm for the generation of trial solutions for any set of equations cannot be directly stated. It is necessary to understand the physics of the problem under consideration to be able to write an appropriate trial solution generation scheme. Therefore, for this discussion the system of equations generated by making a finite difference approximation of the steady state, one-dimensional, heat conduction equation in non-dimensional form [7]

$$\frac{d^2X}{dx^2} = -u'''(x), \quad 0 \leq x \leq 1 \quad (3.1)$$

with boundary conditions

$$X(0) = T_S \quad (3.2)$$

and

$$X(1) = T_F \quad (3.3)$$

will be addressed.

After the finite difference approximation [6] of the derivative in Equation (3.1) is made, and assuming Δx is unity, the [K] matrix of Equation (2.2) has the tridiagonal form

$$\begin{bmatrix} -2 & 1 & 0 & \dots & & \\ 1 & -2 & 1 & 0 & \dots & \\ 0 & 1 & -2 & 1 & 0 & \dots \\ \vdots & & \ddots & \ddots & \ddots & \\ & & & \dots & 0 & 1 & -2 \end{bmatrix} \quad (3.4)$$

The $\{X\}$ matrix of Equation (2.2) contains the unknown temperatures $(\bar{X}_2, \dots, \bar{X}_{n-1})$ corresponding to nodal temperatures of the finite difference model of the problem where n is the number of nodes. The boundary surface temperatures T_S and T_F are assigned nodal temperatures \bar{X}_1 and \bar{X}_n , respectively.

The right hand matrix, $\{F\}$, of Equation (2.2) contains the known boundary temperatures and the heat generation distribution if present:

$$\{F\} = \begin{Bmatrix} \bar{X}_1 - u''''(2) \\ -u''''(3) \\ \vdots \\ -u''''(n-2) \\ \bar{X}_n - u''''(n-1) \end{Bmatrix} \quad (3.5)$$

At iteration level i of the new method after $\{X_i\}$ is known, consider a correction vector $\{x_i^1\}$ such that along with $\{X_i\}$ result in

$$[K]\{X_i + x_i^1\} = \{F\}. \quad (3.6)$$

Rewriting Equation (3.6) as

$$[K]\{X_i\} + [K]\{x_i^1\} = \{F\} \quad (3.7)$$

and using Equation (2.4) results in

$$[K]\{x_i^1\} = -\{e_i\}. \quad (3.8)$$

The matrix $\{e_i\}$ in Equation (3.8) is equivalent in purpose to the $\{F\}$ matrix in Equation (2.2), and therefore, also equivalent to Equation (3.5). But in order to make the combined solution of Equation (3.6) satisfy the original boundary conditions, Equation (3.2) and (3.3), the boundary conditions contained in the $\{e_i\}$ matrix of Equation (3.8), $\bar{x}_{i,1}^1$ and $\bar{x}_{i,n}^1$, must both be zero. Therefore,

$$[K]\{x_i^1\} = -\{e_i\} \quad (3.8)$$

has boundary conditions

$$\bar{x}_{i,1}^1 = \bar{x}_{i,n}^1 = 0. \quad (3.9)$$

By reversing the finite difference approximation procedure, the following differential equation results

$$\frac{d^2 x^1}{dx^2} = -e^{111}(x), \quad 0 \leq x \leq 1 \quad (3.10)$$

with boundary conditions

$$x^1(0) = x^1(1) = 0. \quad (3.11)$$

The $\{x_i^1\}$ matrix can be thought of as the temperature distribution resulting from the heat generation field $\{e_i\}$ of Equation (3.8) just as $\{X\}$ is the solution to the original heat generation field $u^{111}(x)$ in

Equation (3.1). In other words, the error at each node is considered to be a heat source or sink with a magnitude equal to the error at that node, and $\{x_i^1\}$ is the temperature distribution resulting from this heat source/sink field. If $\{x_i^1\}$ could be determined efficiently, then there is little reason why $\{X\}$ could not be determined with the same method, thus completing the problem. But $\{x_i^1\}$ in some cases cannot be determined efficiently; therefore, a routine is presented that approximates $\{x_i^1\}$ with a series of vectors that will respectively become $[x_{i+1,2}]$, $[x_{i+1,3}]$, ..., $[x_{i+1,m}]$, along with $\{X_i\}$ as trial solution $[x_{i+1,1}]$ in the approximation of $\{X_{i+1}\}$.

By linearly superimposing the individual temperature distributions caused by each heat source/sink, the $\{x_i^1\}$ matrix can be approximated. To greatly simplify the approximation, boundary effects will be ignored and the region will be treated as if it were infinite. One condition that will be maintained is that no error in temperature exists at nodes of known temperature. The magnitude of the heat source/sink will be equal to the error at that node as previously stated, and the heat flow associated with each heat source/sink will be symmetric in about node j except where boundary interference occurs. Thus the temperature due to a single source will have a magnitude of an unknown constant, c , multiplying the magnitude of the heat source/sink at the node j , and the effect will be assumed to be negligible at nodes a distance further

away than D from node j . The node that is at, or nearest to the limiting distance D but not over D from node j , will have coordinate position $j \pm d$. The choice of D will affect the convergence rate and will be investigated in the next section.

First consider the case where the error matrix associated with the approximate solution $\{X_i\}$ of iteration level i has only one term at node j and it has magnitude $\bar{e}_{i,j}$. The resulting temperature at node j , $\bar{x}_{i,j}^1$, would be $c\bar{e}_{i,j}$ as previously assumed. The profile would be symmetric with respect to node j and extend outward with decreasing intensity to a distance D from node j . The entire temperature profile resulting from heat generation at only node j would be

$$\bar{x}_{i,k}^1 = c\bar{e}_{i,j}\theta(k-j), \quad (3.12)$$

at node point k where

$$k=j-d, \dots, j-1, j, j+1, \dots, j+d.$$

The function θ describes the shape of the resulting temperature profile as a function of nodal distance and has the value of unity at $\theta(0)$ and is zero for nodal distances larger than d .

For the case of several values in the error matrix of the approximate solution $\{X_i\}$, the resulting temperature at any node j , $\bar{x}_{i,j}^1$, can be written by superimposing the respective temperature profiles of neighboring heat sources/sinks

$$\begin{aligned} \bar{x}_{i,j}^1 &= ce_{i,j-d} \theta(d) + \dots + ce_{i,j-1} \theta(1) & (3.13) \\ &+ ce_{i,j} \theta(0) + ce_{i,j+1} \theta(1) + \dots + ce_{i,j+d} \theta(d) \end{aligned}$$

By symmetry

$$\theta(k) = \theta(-k), \quad k=d, \dots, 1, 0. \quad (3.14)$$

Equation (3.12) can be rewritten by using Equation (3.14) as

$$\begin{aligned} \bar{x}_{i,k}^1 &= c\theta(d)(\bar{e}_{i,j-d} + \bar{e}_{i,j+d}) + \dots + & (3.15) \\ &c\theta(1)(\bar{e}_{i,j-1} + \bar{e}_{i,j+1}) + c\theta(0)\bar{e}_{i,j}. \end{aligned}$$

By defining

$$\begin{aligned} (\bar{e}_{i,j-k} + \bar{e}_{i,j+k}) &= \Sigma \bar{e}_{i,j \pm k}, & (3.16) \\ &k=d, \dots, 1, 0 \end{aligned}$$

and grouping all the unknowns into one term

$$c\theta(k) = \alpha_k, \quad k=d, \dots, 1, 0, \quad (3.17)$$

where

$$c\theta(0) = \alpha_0 = \alpha_e, \quad (3.18)$$

Equation (3.15) can be written in final form as

$$\bar{x}_{i,j}^1 = \alpha_e e_{i,j} + \alpha_1 \Sigma e_{i,j \pm 1} + \dots + \alpha_D \Sigma e_{i,j \pm d}. \quad (3.19)$$

Equating the expression in Equation (3.19) to $\{x_i^1\}$ in Equation (3.6) defines the trial solutions as

$$\begin{aligned}
[X_{i+1,2}] &= [e_{i,j}], \\
[X_{i+1,3}] &= [\Sigma e_{i,j\pm 1}], \\
[X_{i+1,4}] &= [\Sigma e_{i,j\pm 2}], \\
&\vdots \\
[X_{i+1,m}] &= [\Sigma e_{i,j\pm d}],
\end{aligned}
\tag{3.20}$$

where $e_{i,j}$ is the error of the approximate solution $\{X_i\}$ at matrix position j , and setting the α 's of Equation (3.19) equal to the unknown weighting coefficients of Equation (2.3), results in the following expression of $\{X_{i+1}\}$

$$\begin{aligned}
\{X_{i+1}\} &= \alpha_{LB} \{X_i\} + \alpha_e \{e_{i,j}\} + \alpha_1 \{\Sigma e_{i,j\pm 1}\} \\
&\quad + \dots + \alpha_d \{\Sigma e_{i,j\pm d}\},
\end{aligned}
\tag{3.21}$$

where α_{LB} is the unknown weighting coefficient of the last best solution approximation from the previous iteration.

Consider the following problem as a demonstration of the trial solution generation scheme.

$$\frac{d^2 X}{dx^2} = -u''''(x) \quad 0 < x < 5
\tag{3.22}$$

Boundary conditions:

$$X(0) = X(5) = 0
\tag{3.23}$$

The function $u'''(x)$ is defined as

$$u''' = \begin{cases} A, & 0 \leq x \leq 3.5 \\ 2A, & 3.5 \leq x \leq 5 \end{cases} \quad (3.24)$$

By writing Equation (3.22) in finite difference form [6]

$$\frac{x_{i-1} - 2x_i + x_{i+1}}{(\Delta x)^2} = -A_i \quad (3.25)$$

and using a grid of six nodal points with two specified at the boundary (Figure 3.1) making Δx equal unity, the following matrix is generated

$$\begin{bmatrix} -2 & 1 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 0 & 0 & 1 & -2 \end{bmatrix} \begin{Bmatrix} x_2 \\ x_3 \\ x_4 \\ x_5 \end{Bmatrix} = - \begin{Bmatrix} A \\ A \\ A \\ 2A \end{Bmatrix} \quad (3.26)$$

Adopting the notation from the previous section:

$$[K]\{X\} = \{F\} \quad (3.27a)$$

$$[K] = \begin{bmatrix} -2 & 1 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 0 & 0 & 1 & -2 \end{bmatrix} \{X\} = \begin{Bmatrix} x_2 \\ x_3 \\ x_4 \\ x_5 \end{Bmatrix} \{F\} = - \begin{Bmatrix} A \\ A \\ A \\ 2A \end{Bmatrix} \quad (3.27b)$$

At the initial iteration the algorithm, Equation (3.21), does not apply because it is necessary to have the previous approximate solution

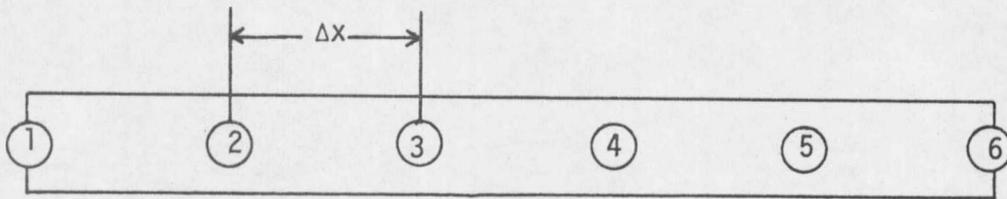


Figure 3.1 Nodal Grid for Equation (3.22)

and its residual matrix. These, of course, do not exist. Therefore, to start the method the following initial approximation was made

$$\{X_0\} = \begin{Bmatrix} A/2 \\ A/2 \\ A/2 \\ A/2 \end{Bmatrix} \quad (3.28)$$

The error matrix and associated variance are determined from Equations (2.4) and (2.5)

$$e_0 = \begin{bmatrix} -2 & 1 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 0 & 0 & 1 & -2 \end{bmatrix} \begin{Bmatrix} A/2 \\ A/2 \\ A/2 \\ A/2 \end{Bmatrix} + \begin{Bmatrix} A \\ A \\ A \\ 2A \end{Bmatrix} \quad (3.29)$$

$$e_0 = \begin{Bmatrix} A/2 \\ A \\ A \\ 3A/2 \end{Bmatrix} \quad (3.30)$$

$$V_0 = e_0^t e_0 = 4.5A^2 \quad (3.31)$$

Using the method of trial solution generation explained above, the example problem was solved with D and A equal to 1 which resulted in the following algorithm for $\{X_{i+1}\}$

$$\{X_{i+1}\} = \alpha_{i+1, LB} \{X_i\} + \alpha_{i+1, e} [e_{i, j}] + \alpha_{i+1, l} [\sum e_{i, j \pm 1}] \quad (3.32)$$

Four iterations were required in double precision to reach a variance less than 0.000001 with the following solution

$$\{X\} = \begin{Bmatrix} 0 \\ 2.200006 \\ 3.399986 \\ 3.599968 \\ 2.799987 \\ 0 \end{Bmatrix} \quad (3.33)$$

with a final variance of 2.156×10^{-9} . Appendix B contains the details of the four iterations. The exact solution to Equation (3.22) is

$$\{X\} = \begin{Bmatrix} 0 \\ 2.2 \\ 3.4 \\ 3.6 \\ 2.8 \\ 0 \end{Bmatrix} \quad (3.34)$$

The solution obtained by the new method, Equation (3.33), was to have an average absolute error of 10^{-4} by Equation (2.7). By using the

actual final variance of Equation (3.33) in Equation (2.7), the predicted absolute average error was 1.47×10^{-5} . The actual average absolute error was 1.625×10^{-5} .

The success of this particular trial solution generation scheme and the final method of collecting them into an approximate solution, Equation (2.24), suggests their continued use in heat conduction problems. In the next section, this new iterative procedure will be used to solve two different conduction problems to determine its performance as compared to the performance of existing methods.

CHAPTER IV

APPLICATION AND RESULTS

The first problem to be considered in this section is a steady state, three-dimensional heat conduction problem. Its presentation will demonstrate the effects of using different values for D , the limiting effect distance in the approximation of $\{X_{i+1}\}$ in Equation (3.21). Various values of D were investigated and by using the execution time of the new method as an indicator, an optimum value of D was established. The same problem was solved by an existing method for a comparison of the execution times of the different methods.

A transient, three-dimensional heat conduction problem was solved by using the optimum value of D previously determined to further demonstrate the performance of the new method. Again, the results of the new method were compared to another existing routine solving the same problem.

Problem One

The elliptical partial differential equation to be solved is

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} = 0 \quad (4.1)$$

where T , x , y , and z are non-dimensional variables for temperature and three spacial coordinates. The geometry is a cube of face length $2IN$ located concentrically in a larger cube of face length $2N$. The inner cube is maintained at a temperature of unity while the outermost surface of the outer cube is set at zero temperature. By using the

symmetry of the problem, only a sixteenth of the composite cube need be considered (Figure 4.1).

The problem is formally stated as: Solve

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} = 0 \quad (4.1)$$

for the region

$$0 \leq z \leq 1 \quad (4.2a)$$

$$0 \leq y \leq 1 \quad (4.2b)$$

$$0 \leq x \leq z \quad (4.2c)$$

with boundary conditions

$$T(x, y, 1) = 0 \quad (4.3a)$$

$$T(x, 1, z) = 0 \quad (4.3b)$$

$$T(x, y, \frac{1N}{N}) = 0 \quad (4.3c)$$

$$T(x, \frac{1N}{N}, z) = 0 \quad (4.3d)$$

$$\frac{\partial T}{\partial x}(z, y, z) = 0 \quad (4.3e)$$

$$\frac{\partial T}{\partial z}(z, y, z) = 0 \quad (4.3f)$$

A standard finite difference technique in three dimensions [4] was used to approximate the second order derivatives in Equation (4.1), and a central difference approximation was used for the first order derivatives of Equation (4.3). The sixteenth cube-cube region was approximated by a network of nodes: eleven to an edge, giving ten

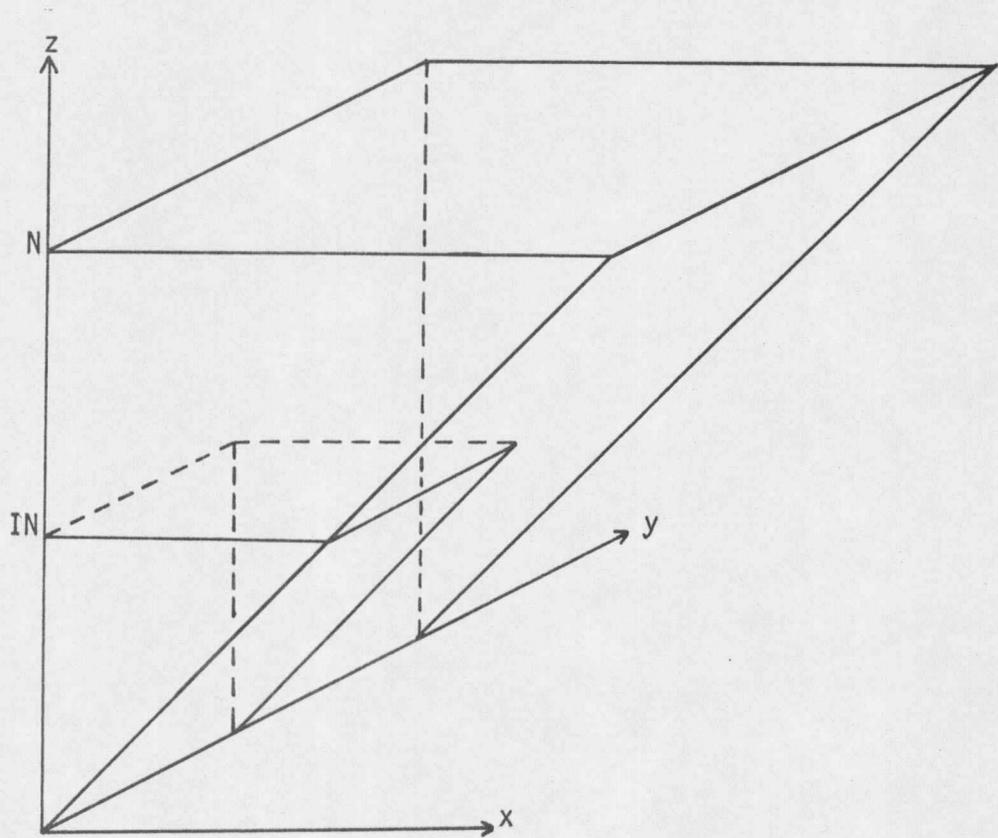


Figure 4.1 Cube-Cube Orientation

nodal spacings and thus $\Delta x = \Delta y = \Delta z = 0.1$. An extra node was included on the faces of symmetry to accommodate the central difference approximation to be taken at such faces.

To determine a measure of the accuracy of the solution, heat fluxes were calculated at the midpoint between the inner cube faces and its outer, parallel, nodal plane; and at the midpoint between the outermost surface of the outer cube and its inner, parallel, nodal plane. The exact solution would yield heat fluxes that are identical at the different surfaces. To non-dimensionalize these quantities, they were divided by the heat flux of concentric spheres with the same boundary conditions and with radii equal to the face length of the cubes. This non-dimensional heat flux was [7]

$$q' = 4\pi r_i r_o / (r_o - r_i) \quad (4.4)$$

In the solution method, different values of D were used beginning with $D=0$, corresponding to two trial solutions, $\{X_i\}$ and $[e_{i,j}]$, and ending with $D=\sqrt{3}$, corresponding to five trial solutions, $\{X_i\}$, $[e_{i,j}]$, $[\Sigma e_{i,j\pm r_1}]$, $[\Sigma e_{i,j\pm r_2}]$, and $[\Sigma e_{i,j\pm r_3}]$. The trial solution $[\Sigma e_{i,j\pm r_1}]$ is the sum of the errors at a distance of one nodal spacing from node j and $j\pm r_1$ are the coordinates in three-dimensions of the nodes that are one nodal space from j . Likewise, $[\Sigma e_{i,j\pm r_2}]$ is the sum of the errors at nodal distance of $\sqrt{2}$ from node j and $j\pm r_2$ are

the coordinates of the nodes that are $\sqrt{2}$ nodal spaces from j . The nodal numbers $j \pm r_3$ are the nodes at a distance of $\sqrt{3}$ from node j . The attempt with four trial solutions, $D=\sqrt{2}$, reached an acceptable solution with a variance of less than 0.000001 in the least execution time. Attempts with less than four trial solutions did not converge rapidly at each iteration due to the poor approximation of the effects of the error matrix. While the attempt of five trial solutions reduced the variance the greatest per iteration, it took a larger number of calculations to generate the additional trial solution and to solve for its weighting coefficient. A more detailed comparison is presented in Table 4.1.

The calculated heat flux and the execution time of the new method were compared to the results obtained by solving the same problem with a Gauss Seidel iteration [2] scheme with a relaxation factor or successive overrelaxation. From the results in Table 4.1, the smallest difference of the calculated heat fluxes on the surface of the inner and outer cube by the new method is on the order of 0.001. The successive overrelaxation method, or SOR, determines convergence when the calculated heat fluxes on the cube surfaces agree to within a preset difference. This difference was set to 0.001 in order to make the results of the SOR method and the new method similar in accuracy. Different relaxation factors ranging from 0.166667 (which made the SOR

Table 4.1 Cube-Cube Results for Various Values of m

NUMBER OF TRIAL SOLUTIONS	NUMBER OF ITERATIONS	AVG. % CHANGE IN V PER ITERATION	HEAT FLUX INNER CUBE	HEAT FLUX OUTER CUBE	% DIFFERENCE IN HEAT BALANCE	USER EXECUTION TIME (MIN)
2	88	17.84	1.5238	1.5265	0.180	1.0758
3	30	43.55	1.5239	1.5261	0.149	0.5720
4	20	57.34	1.5239	1.5260	0.137	0.5405
5	19	57.35	1.5238	1.5261	0.156	0.6748

routine identical to Gauss Seidel iteration) to 3 (which was the optimum over relaxation factor [4]) were used in the SOR method.

The initial estimate of the solution to Equation (4.1) for both methods was a uniform 0.5 temperature distribution.

The details of the various SOR runs are shown in Table 4.2. Steady improvement in the execution time can be seen as the relaxation factor was increased from the standard Gauss Seidel procedure to the optimum over relaxation factor. After the optimum factor was passed the solution diverged. The best execution time of the new method is over six times greater than the SOR method with the optimum relaxation factor. These results can be better shown in a graph of the execution time versus the number of trial solutions used in the new method and the relaxation factor in the SOR method. In Figure 4.2 these results are plotted. Both curves have a concave upward curvature with the minimum execution time corresponding to the best number of trial solutions or optimum relaxation factor. As expected, the optimum relaxation factor produced the best performance. The optimum value of trial solutions is four, both from Figure 4.2 and Table 4.1.

Although the performance of the new method was not better than SOR in the previous problem, it was shown, however, that the optimum value of D in the sense of execution time is $\sqrt{2}$ for three-dimensional heat conduction problems. This information will be used in the

Table 4.2 Cube-Cube Results for Various SOR Factors

SOR FACTOR	NUMBER OF ITERATIONS	HEAT FLUX INNER CUBE	HEAT FLUX OUTER CUBE	% DIFFERENCE IN HEAT BALANCE	USER EXECUTION TIME (MIN)
0.166667 (Gauss Seidel)	105	1.5241	1.5250	0.06	0.2468
0.2	70	1.5241	1.5250	0.06	0.1678
0.25	32	1.5240	1.5248	0.06	0.0871
0.3 (optimum)	29	1.5223	1.5229	0.06	0.0820
0.35	DIVERGED				
0.40	DIVERGED				

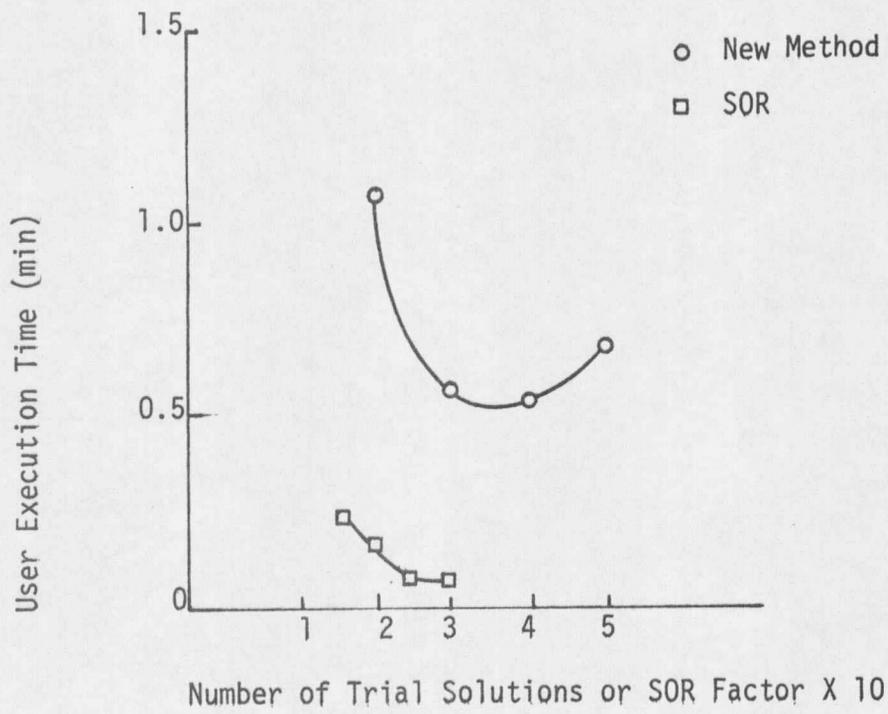


Figure 4.2 Execution Time of Different Numbers of Trial Solutions and Different Relaxation Factors

following problem which is a case where the new method proves to be superior over an existing technique.

Problem Two

This time a parabolic partial differential equation of the form

$$\frac{\partial T}{\partial \tau} = \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \quad (4.5)$$

for the cube region $0 < x < 1$, $0 < y < 1$, and $0 < z < 1$, where T , τ , x , y , and z are all non-dimensional variables representing temperature, time, and three space coordinates, respectively, will be considered. The boundary conditions of Equation (4.4) are

$$T = 0 \text{ at } x=1 \text{ or } y=1 \text{ or } z=1 \quad (4.6a)$$

$$\frac{\partial T}{\partial x} = 0 \text{ at } x=0 \quad (4.6b)$$

$$\frac{\partial T}{\partial y} = 0 \text{ at } y=0 \quad (4.6c)$$

$$\frac{\partial T}{\partial z} = 0 \text{ at } z=0 \quad (4.6d)$$

and the initial condition is

$$T = 1 \text{ at } \tau=0. \quad (4.7)$$

This cube was approximated by a nodal network consisting of $11 \times 11 \times 11$ nodes. Extra nodes were required at the insulated faces as a central difference was used to approximate the first order derivatives (Equation 4.6) and the Crank Nicolson Method [6] was employed to approximate the parabolic equation (Equation 4.5). For each time step

the solution to the previous time was used as the first guess at the solution to new time level. Results were determined for three elapsed non-dimensional times, $\tau=0.1, 0.5,$ and $1.0,$ by using various time increments $\Delta t.$

The same problem was solved by Allada and Quon [8] and in their paper various methods were investigated. Their results showed that an Alternating Direction Explicit Procedure (ADEP) was possibly an order of magnitude faster than Alternating Direction Implicit Procedure (ADIP), and the Brian-Douglas-Rachford method; therefore, ADEP was used for comparison in this problem.

All the trials began with an initial guess of a uniform distribution of temperature equal to 1 and the results were compared to the analytical solution [7]. All pertinent data of the computer runs for each method are in Tables 4.3 and 4.4. Graphs of execution time versus the accuracy of the solution are in Figures 4.3 - 4.5 for the elapsed times 0.1, 0.5, and 1.0.

For elapsed times, $\tau,$ of 0.1 (Figure 4.3 and Table 4.4) the ADEP method consistently determined a solution that had an average percent error slightly above 0.26 percent except for the case of a time step of 0.01 which proved too large to maintain accuracy. As smaller time steps for ADEP were considered, a general pattern of increasing error was established probably due to the accumulation of round-off error for increasing numbers of iterations.

Table 4.3 Summary of Transient Problem Results for New Method

TIME STEP Δt	NUMBER OF TIME STEPS	ELAPSED TIME, τ	AVERAGE % ERRRR	USER EXECUTION TIME (MIN)
0.02	5	0.1	6.2324	1.5733
0.0125	8	0.1	0.6701	1.7312
0.01	10	0.1	0.4401	1.6987
0.005	20	0.1	0.2843	1.8261
0.004	25	0.1	0.2805	2.1163
0.0025	40	0.1	0.2804	2.9611
0.002	50	0.1	0.2813	3.6382
0.025	20	0.5	2.3513	3.7960
0.02	25	0.5	0.5189	3.6436
0.0125	40	0.5	0.1202	3.6792
0.01	50	0.5	0.0264	3.8368
0.005	100	0.5	0.1008	6.0031
0.004	125	0.5	0.1162	7.3202
0.002	250	0.5	0.1366	14.0328

Table 4.3 (continued)

TIME STEP Δt	NUMBER OF TIME STEPS	ELAPSED TIME, τ	AVERAGE % ERROR	USER EXECUTION TIME (MIN)
0.05	20	1.0	>999.9	6.9492
0.04	25	1.0	247.3470	4.7518
0.025	40	1.0	1.5650	4.8632
0.02	50	1.0	0.4408	4.9559
0.0125	80	1.0	0.4247	5.7388
0.01	100	1.0	0.5994	6.4204
0.005	200	1.0	0.8385	11.1948

Table 4.4 Summary of Transient Problem Results for ADEP

TIME STEP Δt	NUMBER OF TIME STEPS	ELAPSED TIME, τ	AVERAGE % ERROR	USER EXECUTION TIME (MIN)
0.01	10	0.1	24.2707	0.1139
0.001	100	0.1	0.2672	0.5612
0.0005	200	0.1	0.2606	1.0471
0.0002	500	0.1	0.2784	2.5572
0.0001	1000	0.1	0.2818	5.0937
0.001	500	0.5	1.2727	2.5725
0.0005	1000	0.5	0.4251	5.0575
0.00025	2000	0.5	0.2136	10.0280
0.0002	2500	0.5	0.1883	12.5557
0.000125	4000	0.5	0.1336	20.0945
0.0001	5000	0.1	0.1545	25.0453
0.002	500	1.0	11.1389	2.5424
0.001	1000	1.0	3.3909	4.9892
0.0005	2000	1.0	1.5281	9.8901
0.00025	4000	1.0	1.0701	19.7930

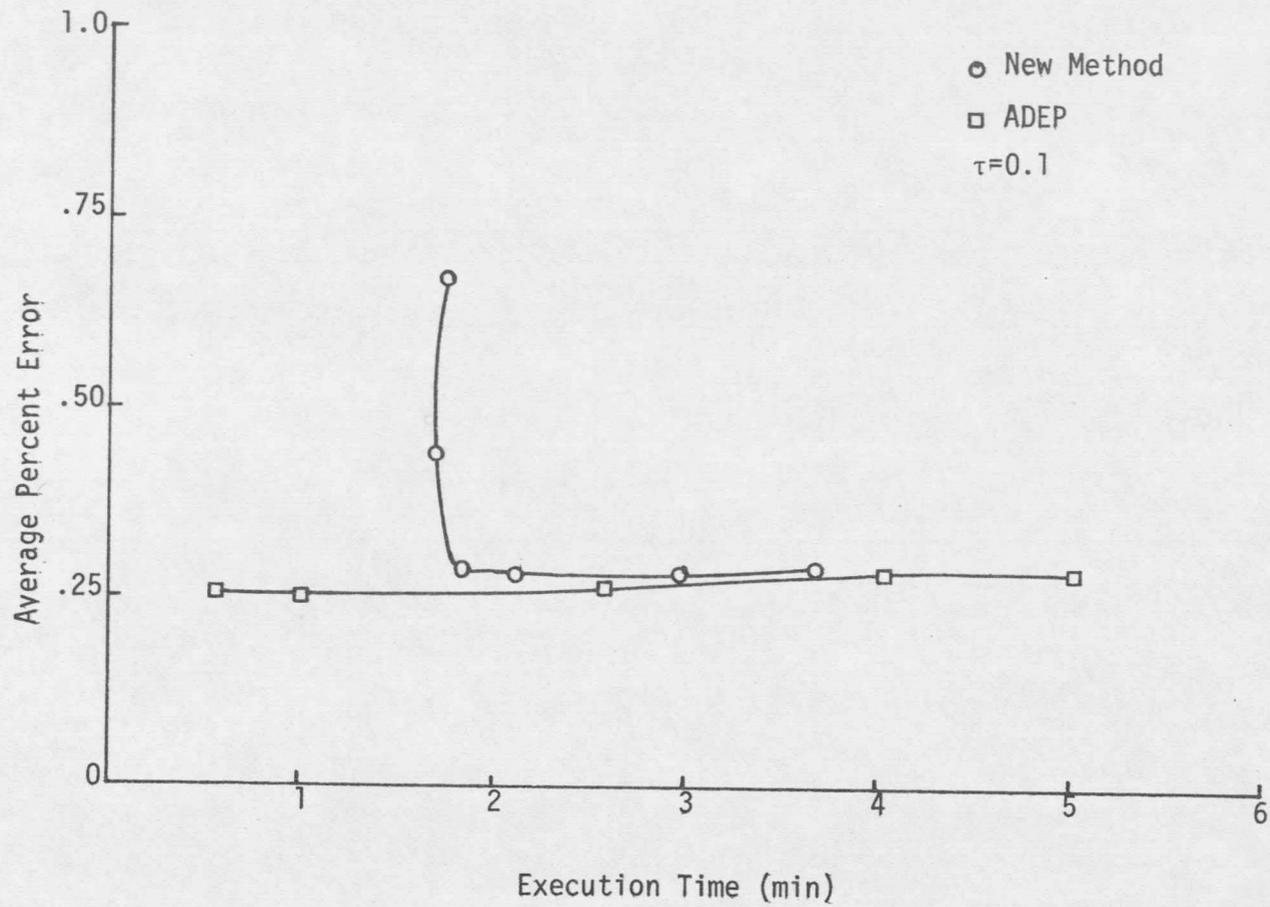


Figure 4.3 ADEP versus New Method at $\tau=0.1$

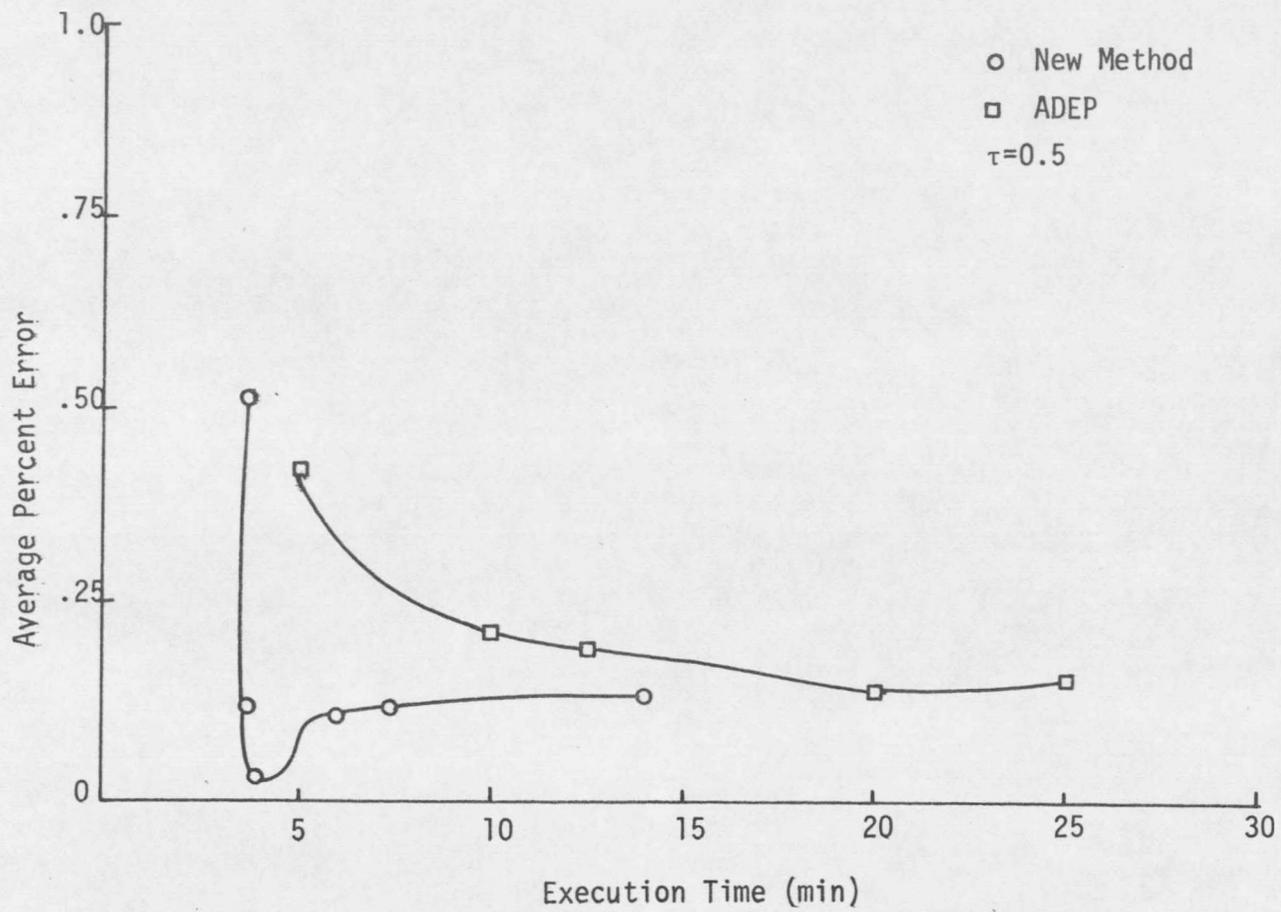


Figure 4.4 ADEP versus New Method at $\tau=0.5$

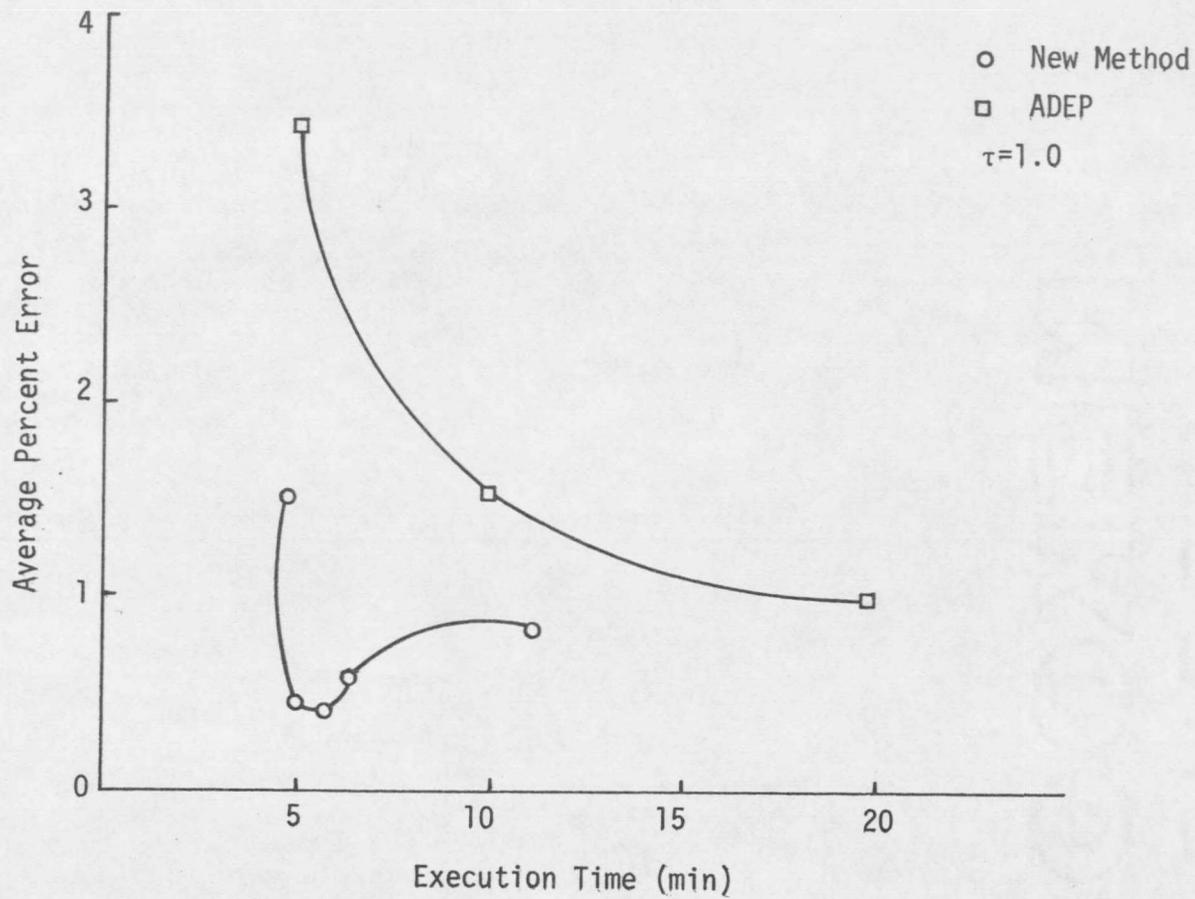


Figure 4.5 ADEP versus New Method at $\tau=1.0$

The graph of the new method's performance (Figure 4.3) established an L-shaped character which became apparent in all its performance curves indicating that once a time step is reached that produces a maximum accuracy, further refinements of the time step did not produce better accuracies in less time. The new method was able to reach the accuracy of the ADEP method but because the elapsed time is small, 0.1 for this case, the results resembled those found for a steady state problem--that is, the existing method being superior in execution time for a given accuracy over the new method. But it is important to note that the new method was able to produce accurate solutions at large time step values, a point that will become even more advantageous for the new method at larger elapsed times.

The superiority of the new method became quite apparent at the elapsed time 0.5. In Figure 4.4 and Table 4.4 it can be seen that the new method's performance is again L-shaped with a noticeable dip as compared to Figure 4.3. The dip is explained by the variance being much lower than the desired value of 0.000001. The lower variance was achieved because the next to the last iteration produced a variance slightly above the desired value which required another iteration that reduced the variance considerably below the desired level and this produced a more accurate solution. The new method reached an extremely accurate (0.0264% error) answer in less than four minutes of

execution time with a time step of 0.0125 and 40 iterations. The ADEP method, restricted to small time steps for better accuracy, reached its best accuracy (0.1336% error) in just over twenty minutes with a time step of 0.000125 and 4000 iterations.

Finally, at elapsed time 1.0 (Figure 4.5) the new method's performance is completely in the envelope of ADEP's performance. By using much larger time steps, the new method benefits in fewer iterations meaning less time and less accumulation of round-off errors. The new method was able to reach accuracies beyond those ever attainable by ADEP.

All computer runs were done in double precision on a Xerox Sigma 7 computer. A flowchart of the new method is shown in Figure 4.6.

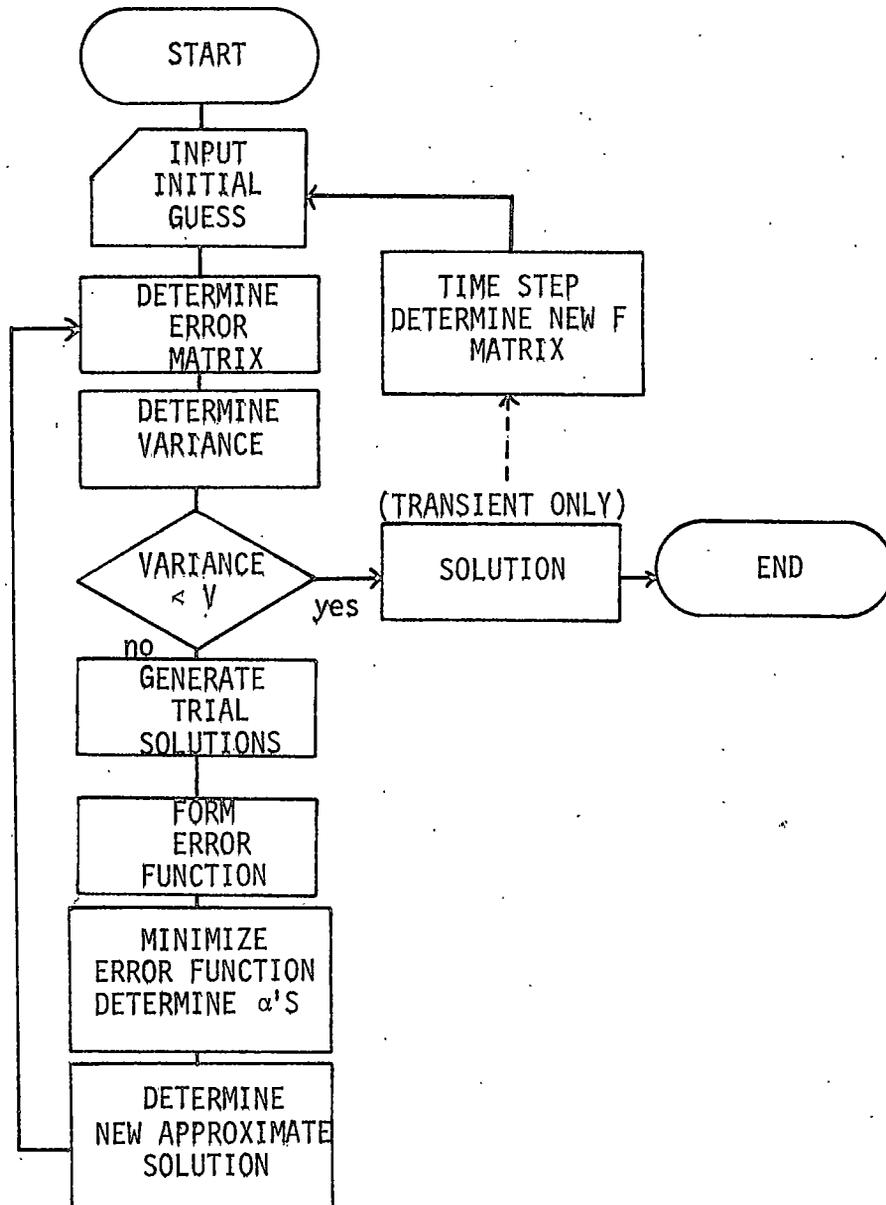


Figure 4.6 Computer Flowchart for New Method

CHAPTER V

CONCLUSION

The superiority of the new method appears to lie in solving transient type problems. This is apparent for two reasons: (1) the ability to operate with large time steps while still maintaining accuracy, and (2) rapid convergence of the method itself. Larger time steps mean less execution time, fewer iterations and smaller accumulation of round-off errors. All are definite advantages.

The rapid convergence is brought about by the method itself. Using the solution of the previous time level as the initial guess for the next time level is a very good estimation for transient type problems. Therefore, the method often corrects itself in just one iteration and thus converges rapidly to the solution at the desired time level. In steady state problems the method would require a very good first estimate of the solution in order to be comparable to existing techniques.

LITERATURE CITED

LITERATURE CITED

1. Blacketter, D. O., R. O. Warrington, M. S. Henry, and E. R. Garner, "A New Iterative Method for Solving Simultaneous Linear Equations," proceedings, Third IMACS International Symposium, June 20-22, 1979.
2. Hestenes, M. R., and E. Stiefel, "Methods of Conjugate Gradients for Solving Linear Systems," Journal of Research of the National Bureau of Standards, Vol. 49, No. 6, Dec., 1952.
3. Stewart, G. W., "Conjugate Direction Methods for Solving Systems of Linear Equations," Numerische Mathematik 21, 285-297, 1973.
4. Rust, B. W., and W. R. Burrus, Mathematical Programming and the Numerical Solution of Linear Equations, New York: American Elsevier Publishing Company, 1972.
5. Golub, G., "Numerical Methods for Solving Linear Least Squares Problems," Numerische Mathematik 7, p. 206-216, 1965.
6. Carnahan, B., H. A. Luther, and S. O. Wilkes, Applied Numerical Methods, New York: John Wiley & Sons, 1969.
7. Kreith, F., Principles of Heat Transfer, fifth edition, New York: Intext Educational Publishers, 1973.
8. Allada, S. R. and D. Quon, "A Stable, Explicit Numerical Solution of the Conduction Equation for Multi-Dimensional Non-homogeneous Media," Chemical Engineering Progress Symposium Series, Vol.62, No.64.
9. Newman, A. B., "Drying of Porous Solids: Diffusion Calculations," Transactions American Institute of Chemical Engineers, Vol. 27, p. 310, 1931.

APPENDICES

APPENDIX A

EXAMPLE OF THE NEW METHOD SHOWING CONSEQUENCES OF DIFFERENT TRIAL SOLUTION SELECTION

To illustrate the theory of the new method, consider the following problem.

$$\begin{bmatrix} 1 & 1 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{cases} \bar{x}_1 \\ \bar{x}_2 \\ \bar{x}_3 \end{cases} = \begin{cases} 2 \\ 3 \\ 1 \end{cases}$$

For an initial guess, select

$$[x_{0,1}] = \begin{cases} 1 \\ 0 \\ 0 \end{cases} \text{ and } [x_{0,2}] = \begin{cases} 0 \\ 1 \\ 1 \end{cases}$$

Thus $n=3$ and $m=2$.

Then equation (2.3) becomes

$$\{X_0\} = \alpha_{0,1}[x_{0,1}] + \alpha_{0,2}[x_{0,2}] = \begin{cases} \alpha_{0,1} \\ \alpha_{0,2} \\ \alpha_{0,2} \end{cases}$$

and

$$KX_0 - F = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{cases} \alpha_{0,1} \\ \alpha_{0,2} \\ \alpha_{0,2} \end{cases} - \begin{cases} 2 \\ 3 \\ 1 \end{cases} = \begin{cases} \alpha_{0,1} + \alpha_{0,2} - 2 \\ \alpha_{0,1} + 2\alpha_{0,2} - 3 \\ \alpha_{0,2} - 1 \end{cases}$$

Now

$$\langle KX_0 - F, KX_0 - F \rangle = (\alpha_{0,1} + \alpha_{0,2} - 2)^2 + (\alpha_{0,1} + 2\alpha_{0,2} - 3)^2 + (\alpha_{0,2} - 1)^2$$

which is equal to the $V_0(\alpha_{0,1}, \alpha_{0,2})$ in Equation (2.5). Forming the partial derivatives according to Equation (2.6) yields

$$\frac{\partial V_0}{\partial \alpha_{0,1}} = 2\alpha_{0,1} + 3\alpha_{0,2} - 5$$

and

$$\frac{\partial V_0}{\partial \alpha_{0,2}} = \alpha_{0,1} + 2\alpha_{0,2} - 3.$$

Thus $\frac{\partial V_0}{\partial \alpha_{0,1}} = 0$ and $\frac{\partial V_0}{\partial \alpha_{0,2}} = 0$ yields the system

$$2\alpha_{0,1} + 3\alpha_{0,2} = 5$$

$$\alpha_{0,1} + 2\alpha_{0,2} = 3$$

with solution

$$\alpha_{0,1} = 1, \alpha_{0,2} = 1.$$

That is $(\alpha_{0,1}, \alpha_{0,2}) = (1, 1)$ and thus

$$\{X_0\} = [x_{0,1}] + [x_{0,2}] = \begin{Bmatrix} 1 \\ 1 \\ 1 \end{Bmatrix}.$$

For the second iteration, Equation (2.8) becomes

$$[x_{1,1}] = [x_{0,1}] + [x_{0,2}] = \begin{Bmatrix} 1 \\ 1 \\ 1 \end{Bmatrix}.$$

Select arbitrarily

$$[x_{1,2}] = \begin{Bmatrix} 1 \\ 2 \\ 2 \end{Bmatrix}.$$

In general, if specific information is known, $x_{1,2}$ may be strategically chosen. In absence of such information one might define $x_{1,2}$ to equal $x_{0,2}$. We deviate from this merely for illustrative purposes.

Therefore, following Equations (2.4) - (2.6) we have

$$\{X_1\} = \alpha_{1,1}[x_{1,1}] + \alpha_{1,2}[x_{1,2}] = \begin{Bmatrix} \alpha_{1,1} & \alpha_{1,2} \\ \alpha_{1,1} + 2\alpha_{1,2} \\ \alpha_{1,1} & \alpha_{1,2} \end{Bmatrix},$$

$$KX_1 - F = \begin{Bmatrix} 2\alpha_{1,1} + 3\alpha_{1,2} - 2 \\ 3\alpha_{1,1} + 5\alpha_{1,2} - 3 \\ \alpha_{1,1} + 2\alpha_{1,2} - 1 \end{Bmatrix},$$

$$\begin{aligned}
 V_1(\alpha_{1,1}, \alpha_{1,2}) &= \langle KX_1 - F, KX_1 - F \rangle \\
 &= (2\alpha_{1,1} + 3\alpha_{1,2} - 2)^2 + (3\alpha_{1,1} + 5\alpha_{1,2} - 3)^2 \\
 &\quad + (\alpha_{1,1} + 2\alpha_{1,2} - 1)^2,
 \end{aligned}$$

$$\frac{\partial V_1}{\partial \alpha_{1,1}} = 14\alpha_{1,1} + 23\alpha_{1,2} - 14$$

$$\frac{\partial V_1}{\partial \alpha_{1,2}} = 23\alpha_{1,1} + 38\alpha_{1,2} - 23,$$

and the equations to be solved are

$$14\alpha_{1,1} + 23\alpha_{1,2} = 14$$

$$23\alpha_{1,1} + 38\alpha_{1,2} = 23$$

with solution

$$\alpha_{1,1} = 1, \alpha_{1,2} = 0.$$

Thus

$$\{X_1\} = [X_{1,1}] = \{X_0\} = \begin{Bmatrix} 1 \\ 1 \\ 1 \end{Bmatrix}$$

and the algorithm terminates with the solution

$$\{X_1\} = \begin{Bmatrix} 1 \\ 1 \\ 1 \end{Bmatrix}.$$

If for the above example,

$$[x_{0,1}] = \begin{Bmatrix} 1.50 \\ .60 \\ 1.00 \end{Bmatrix}$$

and

$$[x_{0,2}] = \begin{Bmatrix} -3.00 \\ 2.00 \\ -.70 \end{Bmatrix}$$

and, at the next step

$$[x_{1,2}] = \begin{Bmatrix} 16.83 \\ 11.63 \\ -15.32 \end{Bmatrix}$$

the respective iterations resulted in

$$\{X_0\} = \begin{Bmatrix} 1.09 \\ .95 \\ .93 \end{Bmatrix}$$

and

$$\{X_1\} = \begin{Bmatrix} 1.07 \\ .96 \\ 1.00 \end{Bmatrix}$$

Thus the initial choice of $[x_{0,1}]$ and $[x_{0,2}]$ affects convergence rates.

APPENDIX B

SOLUTION OF EQUATIONS (3.25 - 3.27) AND
RESULTS OF EACH ITERATION

Iteration 1

$$\{X_0\} = \begin{pmatrix} .5000 \\ .5000 \\ .5000 \\ .5000 \end{pmatrix}$$

$$\{e_0\} = \begin{pmatrix} .5000 \\ 1.0000 \\ 1.0000 \\ 1.5000 \end{pmatrix}$$

$$V_0 = 4.500000$$

$$\{X_1\} = \alpha_{1,1} \begin{pmatrix} .5000 \\ .5000 \\ .5000 \\ .5000 \end{pmatrix} + \alpha_{1,2} \begin{pmatrix} .5000 \\ 1.0000 \\ 1.0000 \\ 1.5000 \end{pmatrix} + \alpha_{1,3} \begin{pmatrix} 1.0000 \\ 1.5000 \\ 2.5000 \\ 1.0000 \end{pmatrix}$$

$$\alpha_{1,1} = 1.08888888888889$$

$$\alpha_{1,2} = .95555555555556$$

$$\alpha_{1,3} = .55555555555556$$

Iteration 2

$$\{X_1\} = \begin{pmatrix} 1.5778 \\ 2.3333 \\ 2.8889 \\ 2.5333 \end{pmatrix}$$

$$\{e_1\} = \begin{pmatrix} .1778 \\ .8000 \\ .0889 \\ -.1778 \end{pmatrix}$$

$$V_1 = .711111$$

$$\{X_2\} = \alpha_{2,1} \begin{pmatrix} 1.5778 \\ 2.3333 \\ 2.8889 \\ 2.5333 \end{pmatrix} + \alpha_{2,2} \begin{pmatrix} .1778 \\ .8000 \\ .0889 \\ -.1778 \end{pmatrix} + \alpha_{2,3} \begin{pmatrix} .8000 \\ .2667 \\ .6222 \\ .0889 \end{pmatrix}$$

$$\alpha_{2,1} = 1.14623197950733$$

$$\alpha_{2,2} = .789480848283625$$

$$\alpha_{2,3} = .318434181207391$$

Iteration 3

$$\{X_2\} = \begin{pmatrix} 2.2036 \\ 3.3910 \\ 3.5796 \\ 2.7917 \end{pmatrix}$$

$$\{e_2\} = \begin{pmatrix} -.0162 \\ .0012 \\ .0235 \\ -.0038 \end{pmatrix}$$

$$V_2 = .000829$$

$$\{X_3\} = \alpha_{3,1} \begin{pmatrix} 2.2036 \\ 3.3910 \\ 3.5796 \\ 2.7917 \end{pmatrix} + \alpha_{3,2} \begin{pmatrix} -.0162 \\ .0012 \\ .0235 \\ -.0038 \end{pmatrix} + \alpha_{3,3} \begin{pmatrix} .0012 \\ .0073 \\ -.0027 \\ .0235 \end{pmatrix}$$

$$\alpha_{3,1} = 1.00240758757177$$

$$\alpha_{3,2} = .532382398167053$$

$$\alpha_{3,3} = .150769136554601$$

Iteration 4

$$\{X_1\} = \begin{pmatrix} 2.2005 \\ 3.4009 \\ 3.6004 \\ 2.8000 \end{pmatrix}$$

$$\{e_3\} = \begin{pmatrix} -.0000 \\ -.0010 \\ .0002 \\ .0004 \end{pmatrix}$$

$$V_3 = .000001$$

$$\{X_4\} = \alpha_{4,1} \begin{pmatrix} 2.2005 \\ 3.4009 \\ 3.6004 \\ 2.8000 \end{pmatrix} + \alpha_{4,2} \begin{pmatrix} -.0000 \\ -.0010 \\ .0002 \\ .0004 \end{pmatrix} + \alpha_{4,3} \begin{pmatrix} -.0010 \\ .0001 \\ -.0006 \\ .0002 \end{pmatrix}$$

$$\alpha_{4,1} = .999898107328567$$

$$\alpha_{4,2} = .618637864034680$$

$$\alpha_{4,3} = .228331597335367$$

$$\{X_4\} = \begin{pmatrix} 2.200006 \\ 3.399986 \\ 3.599968 \\ 2.799987 \end{pmatrix}$$

$$V_4 = 2.156087938886816E-09$$

SOLUTION




N378 Horning, Rodney P
H7832 A new iterative method
cop.2 for solving simultaneous
equations ...

DATE	ISSUED TO
11/24/80	1116 R08 4-3305 Dan Arrale


N378
H7832
Cop 2