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

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.

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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
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NOMENCLATURE

Symbol	Description
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)
$\overline{e}_{i,j}$	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)
$\overline{e}'$	the desired average error (Equation 2.7)
e'''	errors viewed as heat generation (Equation 3.10)
$\{F\}$	right hand matrix (Equation 2.2)
$\overline{F}_j$	specific coefficient of $\{F\}$ at matrix position j (Equation 2.1)
$[K]$	general coefficient matrix (Equation 2.2)
$\overline{K}_{j,k}$	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)

Symbol	Description
r_o	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)
$\overline{X}_j$	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)
$\overline{x}'_{i,j}$	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)

Symbol	Description
$\alpha_{i,j}$	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

$$\begin{aligned} \overline{K}_{1,1}\overline{X}_1 + \overline{K}_{1,2}\overline{X}_2 + \ldots + \overline{K}_{1,n}\overline{X}_n &= \overline{F}_1 \\ \overline{K}_{2,1}\overline{X}_1 + \overline{K}_{2,2}\overline{X}_2 + \ldots + \overline{K}_{2,n}\overline{X}_n &= \overline{F}_2 \\ \ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots & \\ \overline{K}_{n,1}\overline{X}_1 + \overline{K}_{n,2}\overline{X}_2 + \ldots + \overline{K}_{n,n}\overline{X}_n &= \overline{F}_n \end{aligned} \tag{2.1}$$

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

$$[K]\{X\} = \{F\} \tag{2.2}$$

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

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

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)

$$[K]\{X_i\} - \{F\} = \{e_i\} \tag{2.4}$$

and the squared residual, or variance, is

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

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

$$\frac{\partial V_i}{\partial \alpha_{i,j}} = 0, \; j=1,m. \tag{2.6}$$

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 mxm 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

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

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:

$$[x_{i+1,1}] = \{X_i\} \tag{2.8}$$

and by selecting the additional trial solutions

$$[x_{i+1,j}], \; j=2,m \tag{2.9}$$

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

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

The preceeding 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

$$V_{i+1} \leq V_i \quad . \tag{2.11}$$

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]

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

with boundary conditions

$$X(0) = T_S \tag{3.2}$$

and

$$X(1) = T_F \tag{3.3}$$

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

$$\begin{bmatrix} -2 & 1 & 0 & \cdots & & \\ 1 & -2 & 1 & 0 & \cdots & \\ 0 & 1 & -2 & 1 & 0 & \cdots \\ \vdots & & \ddots & \ddots & \ddots & \ddots \\ & & & \cdots & 0 & 1 & -2 \end{bmatrix} \tag{3.4}$$

The {X} matrix of Equation (2.2) contains the unknown temperatures ($\overline{X}_2$, ..., $\overline{X}_{n-1}$) 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 $\overline{X}_1$ and $\overline{X}_n$, respectively.

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

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

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

$$[K]\{X_i + x_i'\} = \{F\}. \tag{3.6}$$

Rewriting Equation (3.6) as

$$[K]\{X_i\} + [K]\{x_i'\} = \{F\} \tag{3.7}$$

and using Equation (2.4) results in

$$[K]\{x_i'\} = -\{e_i\}. \tag{3.8}$$

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), $\bar{x}_{i,1}'$ and $\bar{x}_{i,n}'$, must both be zero. Therefore,

$$[K]\{x_i'\} = -\{e_i\} \tag{3.8}$$

has boundary conditions

$$\bar{x}_{i,1} = \bar{x}_{i,n} = 0. \tag{3.9}$$

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

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

with boundary conditions

$$x'(0) = x'(1) = 0. \tag{3.11}$$

The $\{x_i'\}$ 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 $u'''(x)$ 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 $\{x_i'\}$ is the temperature distribution resulting from this heat source/sink field. If $\{x_i'\}$ could be determined efficiently, then there is little reason why $\{X\}$ could not be determined with the same method, thus completing the problem. But $\{x_i'\}$ in some cases cannot be determined efficiently; therefore, a routine is presented that approximates $\{x_i'\}$ 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 $\{x_i'\}$ 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±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, $\bar{x}'_{i,j}$, 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

$$\bar{x}'_{i,k} = c\bar{e}_{i,j}\theta(k-j), \tag{3.12}$$

at node point k where

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

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, $\bar{x}'_{i,j}$, can be written by superimposing the respective temperature profiles of neighboring heat sources/sinks

$$\bar{x}'_{i,j} = ce_{i,j-d}\,\theta(d) + \ldots + ce_{i,j-1}\,\theta(1) \qquad (3.13)$$

$$+ ce_{i,j}\,\theta(0) + ce_{i,j+1}\,\theta(1) + \ldots + ce_{i,j+d}\,\theta(d)$$

By symmetry

$$\theta(k) = \theta(-k),\ k=d,\ \ldots,\ 1,\ 0. \qquad (3.14)$$

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

$$\bar{x}'_{i,k} = c\theta(d)(\bar{e}_{i,j-d} + \bar{e}_{i,j+d}) + \ldots + \qquad (3.15)$$

$$c\theta(1)(\bar{e}_{i,j-1} + \bar{e}_{i,j+1}) + c\theta(0)\bar{e}_{i,j}\ .$$

By defining

$$(\bar{e}_{i,j-k} + \bar{e}_{i,j+k}) = \Sigma\bar{e}_{i,j\pm k}, \qquad (3.16)$$

$$k=d,\ \ldots,\ 1,\ 0$$

and grouping all the unknowns into one term

$$c\theta(k) = \alpha_k,\ k=d,\ \ldots,\ 1,\ 0, \qquad (3.17)$$

where

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

Equation (3.15) can be written in final form as

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

Equating the expression in Equation (3.19) to $\{x'_i\}$ in Equation (3.6) defines the trial solutions as

$$
\begin{aligned}
[x_{i+1,2}] &= [e_{i,j}], \\
[x_{i+1,3}] &= [\Sigma e_{i,j\pm1}], \\
[x_{i+1,4}] &= [\Sigma e_{i,j\pm2}], \\
&\vdots \qquad\qquad \vdots \\
[x_{i+1,m}] &= [\Sigma e_{i,j\pm d}],
\end{aligned}
\tag{3.20}
$$

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 $\{X_{i+1}\}$

$$
\{X_{i+1}\} = \alpha_{LB}\{X_i\} + \alpha_e\{e_{i,j}\} + \alpha_1\{\Sigma e_{i,j\pm1}\} + \ldots + \alpha_d\{\Sigma e_{i,j\pm d}\}, \tag{3.21}
$$

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.

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

Boundary conditions:

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

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

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

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

$$\frac{X_{i-1} - 2X_i + X_{i+1}}{(\Delta x)^2} = -A_i \tag{3.25}$$

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

$$\begin{bmatrix} -2 & 1 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 0 & 0 & 1 & -2 \end{bmatrix} \begin{Bmatrix} X_2 \\ X_3 \\ X_4 \\ X_5 \end{Bmatrix} = - \begin{Bmatrix} A \\ A \\ A \\ 2A \end{Bmatrix} \tag{3.26}$$

Adopting the notation from the previous section:

$$[K]\{X\} = \{F\} \tag{3.27a}$$

$$[K] = \begin{bmatrix} -2 & 1 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 0 & 0 & 1 & -2 \end{bmatrix} \quad \{X\} = \begin{Bmatrix} X_2 \\ X_3 \\ X_4 \\ X_5 \end{Bmatrix} \quad \{F\} = - \begin{Bmatrix} A \\ A \\ A \\ 2A \end{Bmatrix} \tag{3.27b}$$

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

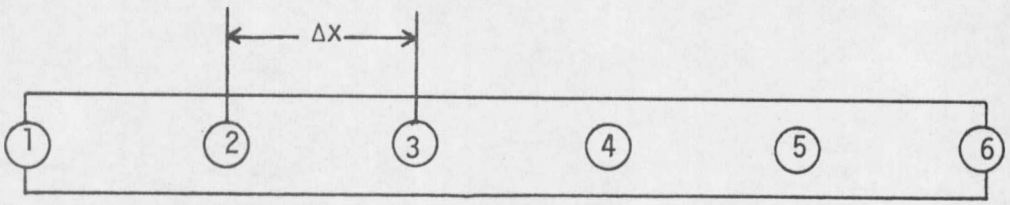

Figure 3.1 Nodal Grid for Equation (3.22)

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

$$\{X_0\} = \begin{Bmatrix} A/2 \\ A/2 \\ A/2 \\ A/2 \end{Bmatrix} \tag{3.28}$$

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

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

$$e_0 = \begin{Bmatrix} A/2 \\ A \\ A \\ 3A/2 \end{Bmatrix} \tag{3.30}$$

$$V_0 = e_0^t e_0 = 4.5A^2 \tag{3.31}$$

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 $\{X_{i+1}\}$

$$\{X_{i+1}\} = \alpha_{i+1,LB}\{X_i\} + \alpha_{i+1,e}[e_{i,j}] + \alpha_{i+1,1}[\Sigma e_{i,j\pm1}] \quad (3.32)$$

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

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

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

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

for the region

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

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

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

with boundary conditions

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

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

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

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

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

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

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