ALGORITHMIC ASPECTS OF TRANSIENT

HEAT TRANSFER PROBLEMS IN STRUCTURES

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ABSTRACT

The application of finite element or finite difference techniques to the solution of transient heat transfer problems in structures often results in a stiff system of ordinary differential equations. Such systems are usually handled most efficiently by implicit integration techniques which require the solution of large and sparse systems of algebraic equations. Most of the computation time required for the solution is spent in assembling and solving these algebraic equations. The present paper is mainly concerned with efficient assembly and solution of these systems using the incomplete Cholesky conjugate gradient algorithm. Several examples are used to demonstrate the advantage of the algorithm over other techniques.

INTRODUCTION

The analysis and design of high speed reentry vehicles such as the space shuttle require the prediction and optimization of the thermal-structural behavior. This means that the analyst needs to solve the heat transfer equation in a structure with complex boundary conditions, irregular geometries and variable thermal properties. The finite element method is one of the more effective approaches available for numerical solution of the transient heat transfer in complex structures. It is therefore expected that finite element systems such as SPAR (Ref. 1) will play a growing role in the analysis and design of such vehicles.

The application of the finite element method to transient heat transfer problems often results in a system of stiff ordinary differential equations (ODE's). Stiff ODE's are characterized by solutions with widely varying time constants. The typical case is when the solution to the homogeneous problem has very small time constants compared to those of the forcing function.

A great deal of effort was devoted in recent years to the development of integration techniques that are suitable for the solution of stiff systems of ODE's. In general, these are variable step size (and, sometimes, variable order) implicit techniques such as the Gear algorithms (Refs. 2,3). The ap-

plication of such techniques to structural heat transfer problems has been recently shown to be very efficient (Ref. 4) compared to explicit algorithms.

The use of implicit integration techniques requires the repeated solution of large systems of algebraic equations. Because of radiation effects and temperature dependent material properties, these equations are nonlinear. These nonlinear equations are solved typically by the Newton Raphson method or its modified variant which replaces them by systems of linear equations. It is the assembly and solution of these large systems of equations which consumes the bulk of the computation time in the solution of a transient heat transfer problem. This topic is also the focus of this paper.

The solution of systems of linear algebraic equations can be handled by direct methods such as Gaussian elimination or by iterative methods such as successive over-relaxation (SOR). Problems in solid mechanics and structures are usually discretized by a finite element method and the associated systems of linear equations solved by elimination techniques. On the other hand, in fluid mechanics problems, finite difference methods are more common and the associated linear equations are solved by iterative techniques. Two reasons for the preference of structural analysts for elimination techniques are worth noting. The first is the ill conditioning which is typical of the systems of linear equations generated by a structural finite element model. This ill conditioning results in very slow convergence rates of iterative solution methods. The second reason is the typically good band structure of the system matrices which results from the use of one and two dimensional finite element models. This property allows efficient solution by elimination using band or skyline solvers.

In applications to transient heat transfer in structures, the finite element codes such as SPAR (Ref. 1) tend to use elimination techniques while finite difference (or lumped parameter) codes such as MITAS (Ref. 5) lean toward the use of iterative techniques. However, neither approach is entirely satisfactory, the iterative methods because of poor convergence and elimination techniques because of poor performance for wide band systems associated with radiation interconnectivities and three dimensional elements.

A promising new technique which is a cross between elimination techniques and iterative techniques is the incomplete Cholesky conjugate gradient (ICCG) method developed by Meijerink and Van der Vorst (Ref. 6), and extended by Kershaw (Ref. 7) to asymmetric matrices. The method has been successfully applied to finite difference modeled transport problems in plasma physics (Refs. 8-10), to finite difference and finite element modeled boundary value problems (Ref. 11-13), and to finite element modeled groundwater flow problems (Ref. 14).

The present paper is concerned with the implementation of the ICCG method to transient heat transfer problems in structures modeled by finite elements. Because of the repeated need to assemble and solve a similar system of equations. it is possible to reduce the computational effort by preliminary calculations. The ICCG method is compared to a conventional band-matrix elimination technique as well as to iterative techniques. A two dimensional space shuttle frame model and an insulated cylinder are used to demonstrate the efficiency of the method.

Numerical Integration Technique

A discretized transient heat transfer problem is governed by the following system of ordinary differential equations (ODE)

$$C(T,t)\dot{T} = Q(T,t) - K(T,t)T \qquad T(0) \text{ given} \qquad (1)$$

where T is the vector of nodal temperatures, C is the capacitance matrix, K is the total conduction matrix (including radiation and convection effects), Q is the thermal load vector and a dot indicates derivatives with respect to time, t. The dependence of the matrices C and K on time and temperature is due to time and temperature dependent material properties and to radiation. However, the cost of recalculating these matrices whenever T or t is changed is exorbitant, especially when three dimensional finite elements are involved. To alleviate this problem, the integration time is divided into time intervals and the material properties assumed to be constant in each time interval. As a result, in each time interval the matrix C is constant and the only variable part of the matrix K is due to radiation effects.

The ODE system (1) is most efficiently solved by a variable order, variable time step algorithm such as employed in the GEAR package (Ref. 3). However, in the present work, a simple fixed-step mid-difference (Crank Nicholson) algorithm is used. It was shown in Ref. 15 that the performance of the algorithm is quite satisfactory for the problems solved here.

Using a numerical integration algorithm, we evaluate the temperature T at a sequence of time points t_1, t_2, ... Denoting as T_n the approximate solution for $T(t_n)$, the mid-difference algorithm replaces Eq. (1) by

$$\psi(T_n) = 2C\,\frac{T_n - T_{n-1}}{h_n} + K(T_n)T_n + K(T_{n-1})T_{n-1} - Q(T_n,t_n) - Q(T_{n-1},t_n) = 0 \qquad (2)$$

We assume that T_{n-1} has already been calculated so that Eq. (2) is a system of nonlinear algebraic equations for T_n. This system of equations is solved using the Newton Raphson method

$$J[T_n^{(m+1)} - T_n^{(m)}] = -\psi(T_n^{(m)}) \tag{3}$$

where $T_n^{(m)}$ is the m-th iterate and J is the Jacobian

$$J = \frac{\partial \psi}{\partial T_n} \tag{4}$$

If J is not recalculated as a function of $T_n^{(m)}$ but is kept constant, we have the modified Newton method. In the present work J was calculated at the beginning of each time interval (when material properties are updated) and was not updated inside a time interval unless the number of iterations in Eq. (3) exceeded three. As was noted before, the only nonlinearity in Eq. (2) is due to radiation. In the problems considered herein, only radiation to space was considered so that the Jacobian was symmetric and positive definite.

Solution of Linear Equations

Eqs. (3) constitutes a system of linear equations of the form

$$Ax = b \tag{5}$$

where in our case, A is symmetric, positive definite and sparse. Eq. (5) may be solved by elimination techniques or by iterative methods. Herein, several methods of solution were compared. The first is an elimination technique, the Gauss-Doolittle factorization, whereby A is factored as

$$A = LDL^T \tag{6}$$

where L is a lower triangular matrix with diagonal elements equal to one and D is a diagonal matrix. Once A has been factored the solution process proceeds easily.

Most iterative methods proceed by splitting the matrix A into two parts

$$A = M-N \tag{7}$$

and rewriting Eq. (5) as

$$(I - M^{-1}N)x = M^{-1}b \tag{8}$$

From Eq. (8), the following simple fixed point iterative process can be defined

$$x^{m+1} = M^{-1}(b + Nx^{m}) \tag{9}$$

It is desirable to choose M so that it is close to A, so that we get fast convergence (note that if M=A, N=0, a single iteration is enough). On the other hand, we want to choose M so that M^{-1} or its equivalent can be formed cheaply. One well known choice is to take M equal to the diagonal of A (the Jacobi method) and another is to take M equal to the lower triangular part of A (the Gauss Seidel method). Asymptotically, the error in the solution is reduced by a factor equal to the largest eigenvalue of $M^{-1}N$. For most finite element generated matrices, this eigenvalue is very close to one so that convergence is very slow.

A method which is a cross between elimination techniques and iterative techniques is based on obtaining M from an incomplete elimination process. For a positive definite matrix A, the incomplete Cholesky decomposition M is defined as

$$M = LL^{T} \tag{10}$$

where L is a lower triangular matrix with the same sparsity structure as A (that is, no fill-up permitted). The matrix M is a good approximation to the matrix A so that most of the eigenvalues of $M^{-1}N$ are very small. Also, for a very sparse matrix A, the cost in computation time and storage for obtaining L is much smaller than that required for a complete decomposition. However, even though most of the eigenvalues of $M^{-1}N$ are small, it is possible for a few to be close to one so that the convergence of the fixed point iteration, Eq. (9), is slow.

Another method which is sometimes used for the solution of linear equations is the conjugate gradient method.

The conjugate gradient method can be used to solve the system (5) by applying it to minimize the following error measure

$$e = (x-x_e)^{T}A(x-x_e) \tag{11}$$

where x_e is the exact solution and x is the current approximation. Theoretically, the conjugate gradient method should reduce e to zero in no more than n iterations so that it is a deterministic method like Gaussian elimination. Because of round-off error, however, it does not terminate in exactly n iterations and may be regarded as an iterative method. Its convergence, while dependent on the ratio of the maximum to the minimum eigenvalues of A, is more favorable than those of iterative methods like Gauss-Seidel. This is because it tends to eliminate the error components corresponding to extreme eigenvalues

in the first few iterations and attain a high convergence rate later. It has a decided advantage over the standard iterative methods for matrices with very few extreme eigenvalues and a large number of eigenvalues which are bunched together.

Meijerink and Van der Vorst (Ref. 6) put together a very clever combination of all the above techniques which can be very efficient for sparse poorly banded matrices. The idea is to apply the conjugate gradient method to Eq. (8) rather than Eq. (5) where the matrix M is obtained from an incomplete Cholesky decomposition of A, Eq. (10).

Because the matrix M is a good approximation to A, the matrix $I-M^{-1}N$ is close to the unit matrix and most of its eigenvalues are close to one. This provides a good setting for a very fast convergence of the conjugate gradient method.

To take advantage of the incomplete Cholesky conjugate gradient (ICCG) algorithm, sparse matrix storage techniques should be used for the matrix A. The method selected here and its implementation are discussed next.

Matrix Storage, Retrieval and Assembly Technique

The storage and retrieval technique used herein is due to Gustavson (Ref. 16) and Tewarson (Ref. 17). One array EJ is used to store by row all the nonzero elements of the lower triangular part of the Jacobian. Another array IC of the same size contains the column numbers of the entries of EJ. Finally, a third array IA stores the position in EJ of the last nonzero entry in each row so that IA (i)- IA (i-1) is the total number of nonzero elements in the i-th row. A method for generating IC and IA from element data was developed in Ref. 15. The use of the IC and IA arrays is compatible with an efficient implementation of the ICCG algorithm and avoids any operations on zero elements of A or L. It is not convenient, however, for assembling the Jacobian from the individual element matrices.

To expedite the generation and assembly of the Jacobian an additional storage system is used. The element conductivity matrices are calculated and stored for a unit value of the conduction coefficient. For each element matrix, another array IPLACE is generated which stores the destination of each entry of the conductivity matrices in the matrix EJ. During assembly the actual conduction coefficient is computed based on the average temperature of the element and this value is used to multiply the unit matrices. The use of the IPLACE array together with the unit matrices reduces the assembly time for the Jacobian considerably.

Computer Implementation

A computer program that implements the analysis methods denoted SMITT (sparse Matrix Iterative Techniques for Thermal Analysis) was written for the IIT Prime 400 minicomputer (Ref. 15). A parallel program using conventional band matrix storage and Gauss-Doolittle solution was also implemented. The Prime 400 is a virtual memory machine and theoretically each common block or subroutine can have up to 640,000 32 bit words. In practice it was found that

beyond 64,000 words the program did not work, so that this limit controlled the maximum problem size. These programs were exercised on two example programs described in the next section.

RESULTS AND DISCUSSION

Shuttle Orbiter Frame

The first test problem which was used for demonstrating the efficiency of the ICCG algorithm is a shuttle orbiter frame, Fig. 1, tested under transient heat loads by Gallegos (Ref. 18). The finite element model contains 190 grid points and 199 elements, including two dimensional conduction elements and one dimensional radiation elements.

The properties of the aluminum structure and the insulation are functions of temperature (Ref. 18). The band width of the Jacobian is 39.

The problem has been solved for 500 seconds of response time using the ICCG and Gauss Doolittle (GD) algorithms. Material properties were updated every 50 seconds and the integration time step for the Crank-Nicholson method was 25 seconds. The CPU times required for the solution are tabulated in Table 1. It is seen that the ICCG algorithm is about twenty percent faster than Gauss Doolittle. This is remarkable because the problem is only mildly sparse with more than twenty percent of the elements in the band being nonzero.

Insulated Cylinder

For the second test problem, a configuration was sought which was larger (in terms of number of unknown temperatures) than the shuttle frame and exhibited some of the characteristics of an insulated air frame structure. These considerations led to the insulated aluminum cylindrical shell depicted in Fig. 2. The cylinder is 18.3m (720 in.) in length and 2.3 m (90 in.) in diameter. The aluminum is 2.5 cm (1 in.) thick and the insulation is 5.0 cm (2.0 in) thick. The outer surface of the insulation is heated over a region which consists of 1/3 the length of half the circumference. The finite element model consists of a symmetric half of the cylinder and is composed of solid brick elements (K81 elements in SPAR). Additionally, the outer surface of the insulation has quadrilateral radiation elements (R41) which radiate to free space. The time-dependence of the heat load on the cylinder is shown in Fig. 3. In all calculations, material properties of the metal and insulation are temperature dependent and are given in Table 2. The material properties were updated every fifty seconds. The number of nodes, the bandwidth of the Jacobian and the sparsity can be easily changed by varying the number of axial, radial and circumferential elements. Thus the problem is suited for checking the performance of the ICCG algorithm vs. other algorithms for a wide range of these parameters.

The cylinder problem was used to compare the performance of the following algorithms:

(i) Band Gauss-Doolittle elimination

(ii) The conventional static over-relaxation (SOR) method with an over-relaxation parameter of 1.4

(iii) The fixed point iteration given by Eq. (9) with the matrix M given by the incomplete Cholesky, Eq. (11)

(iv) The ICCG algorithm

Three sizes of problems are considered, with the number of nodes being 400,720 and 1100 respectively. For each size results are obtained by keeping the total number of nodes approximately fixed and varying the band width. The total CPU time for calculating 200 seconds of the response is shown in Figure 4 for 400 nodes and in Figure 5 for 720 nodes (the SOR algorithm failed to converge for one point which is shown as a break in the curve).

For the largest problem the core storage requirements for the Gauss-Doolittle elimination could not be met. An explicit formula for predicting the computation time for the Gauss-Doolittle algorithm was devised on the basis of the available data (see Ref. 15). This formula was used to estimate the run time for that algorithm for 1100 nodes. The other three algorithms were actually run for 1100 nodes and the results are given in Figure 6.

From Figures 4, 5, 6, it is clear that the iterative algorithms are quite superior to Gaussian elimination for this problem. The advantage increases with increasing number of nodes and increasing band width. The ICCG algorithm is superior to the other two iterative algorithms. This was due to an average number of iterations of about 2.75 compared to 5 or more for the two other algorithms. An examination of the detailed run times for each subroutine (Ref. 15) revealed that most of the gains over the elimination algorithm were due to difference in the matrix decomposition.

An additional advantage of the iterative algorithms over elimination algorithms results from the insensitivity to band-width. The analyst does not have to worry about the best numbering of the nodes to reduce band width. The sensitivity to nodal numbering is one of the major disadvantages of implicit techniques (when used with Gaussian elimination) compared to explicit integration techniques.

CONCLUDING REMARKS

The system of ordinary differential equations generated by discretizing a transient heat transfer problem in structures is typically stiff. Such systems are most efficiently handled by implicit integration techniques which typically require the solution of large and sparse systems of linear algebraic equations. The generation and solution of these equations account for the major part of the computation in the solution of the differential equations. Traditionally, these algebraic equations are solved either by elimination techniques or by iterative techniques. Herein, it is suggested that a recently developed partial elimination algorithm can be more efficient for three dimensional problems where the algebraic equations are poorly banded.

The partial elimination algorithm - the incomplete Cholesky conjugate gradient (ICCG) algorithm is implemented in a finite element program for transient heat transfer in structures. It is coupled with a sparse matrix assembly and storage systems. The techniques are demonstrated for a two dimensional space shuttle frame and an insulated cylinder modeled by three dimensional finite elements. The ICCG algorithm was compared to the Gauss-Doolittle elimination algorithm as well as to two iterative algorithms. For the cylinder problem the ICCG algorithm was shown to be greatly superior to the elimination algorithm and significantly better than the iterative algorithms. For the well banded two dimensional problem, the ICCG algorithm is still marginally better. The results indicate that the ICCG algorithm has a potential for large saving in computational resources when implemented in computer programs for transient heat transfer in structures.

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Table 1. Solution Time for Shuttle Frame*

DURATION TIME SEC.	GAUSS-DOOLITTLE CPU SEC.	ICCG CPU SEC.
200.	52.54	42.95
500.	128.92	106.12

*Results obtained on a PRIME 400 minicomputer

Table 2. Material Properties for Insulated Cylinder

(a) Insulation: ρ = 160 kg/m^3 (0.00582 lbm/in^3)

T		C		K	
°K	°R	J/kg-°C	Btu/lbm-°R	W/m-°C	Btu/in-s-°R
200	360	523	0.125	0.0381	5.1×10^{-7}
367	660	↓	↓	.0546	7.3
478	860			.0711	9.5
589	1060			.0898	1.2×10^{-6}
700	1260			.112	1.5
811	1460			.142	1.9
922	1660			.180	2.4

(b) Aluminum ρ = 2770 kg/m^3 (0.0101 lbm/in^3)

T		C		K	
°K	°R	J/kg-°C	Btu/lbm-°R	W/m-°C	Btu/in-s-°R
200	360	769	0.184	99.5	0.00133
311	560	861	.206	125.0	.00167
367	660	903	.216	138.0	.00185
422	760	937	.224	154.8	.00207
478	860	974	.233	171.3	.00229
533	960	1012	.242	178.8	.00239
589	1060	1045	.250	181.1	.00242

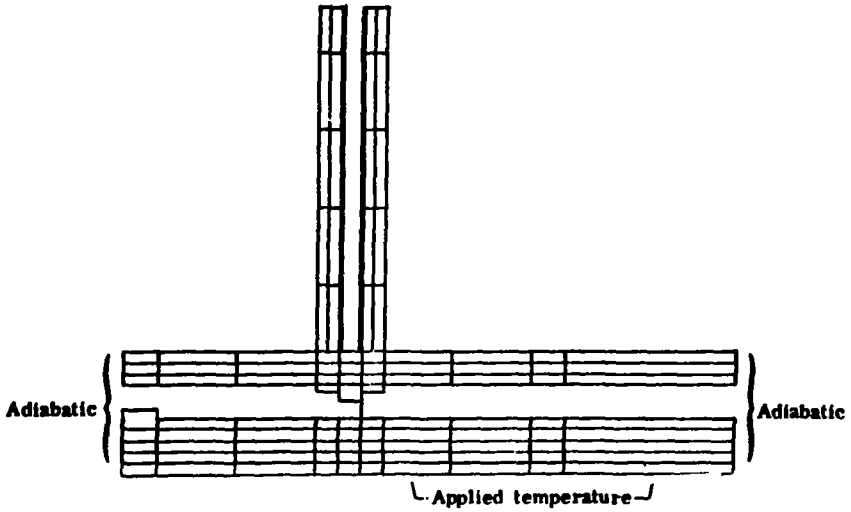

Figure 1.- Finite element model of shuttle frame.

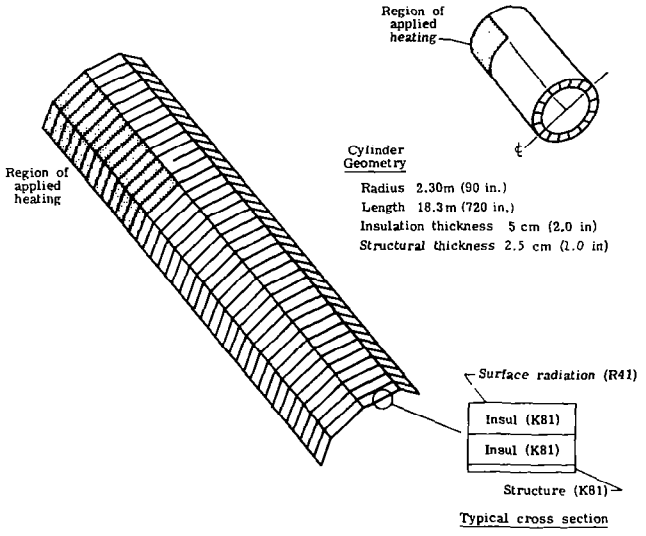

Figure 2.- Finite element model of insulated cylinder.

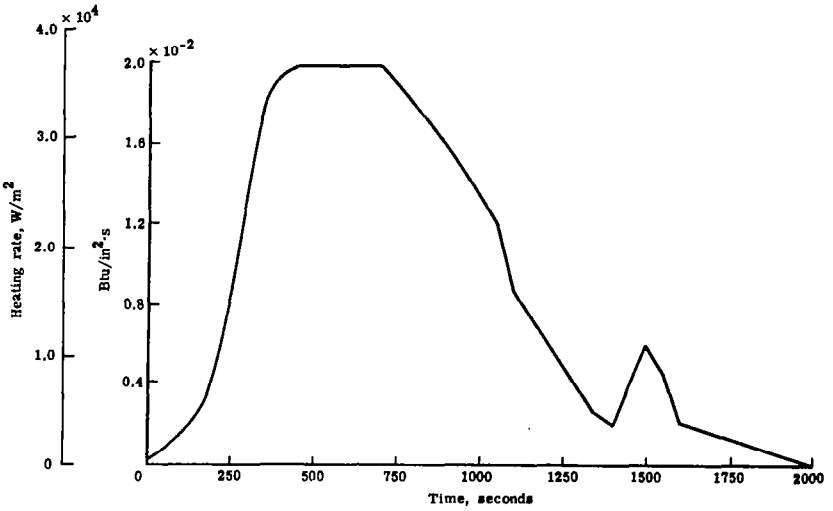

Figure 3.- Heating load at outer surface of insulated cylinder.

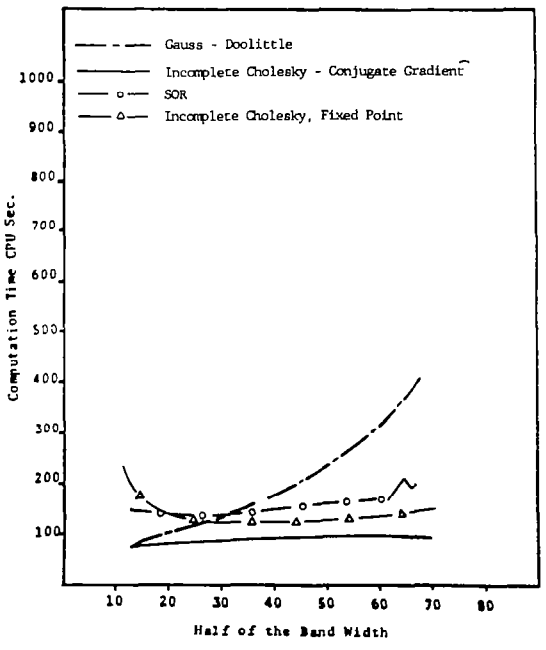

Figure 4.- Effect of Jacobian band width on total computation time for 400 node cylinder models.

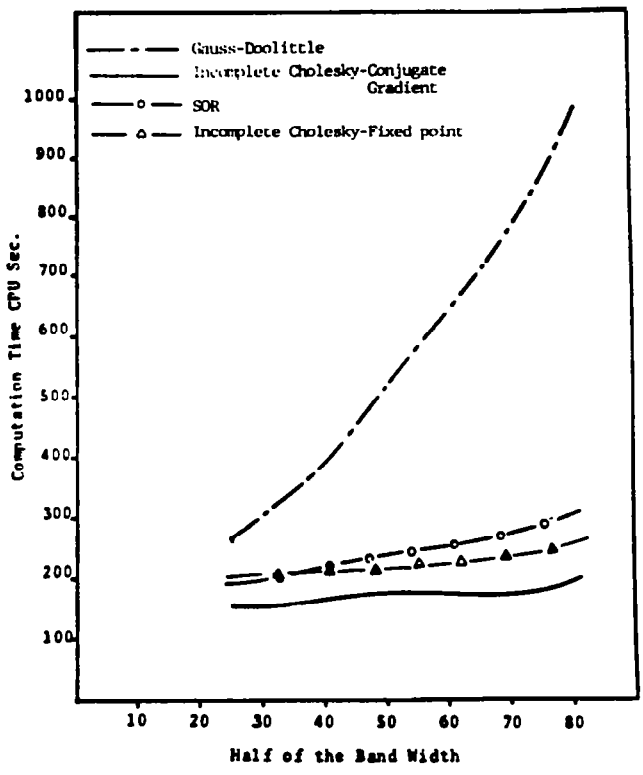

Figure 5.- Effect of Jacobian band width on total computation time for 720 node cylinder models.

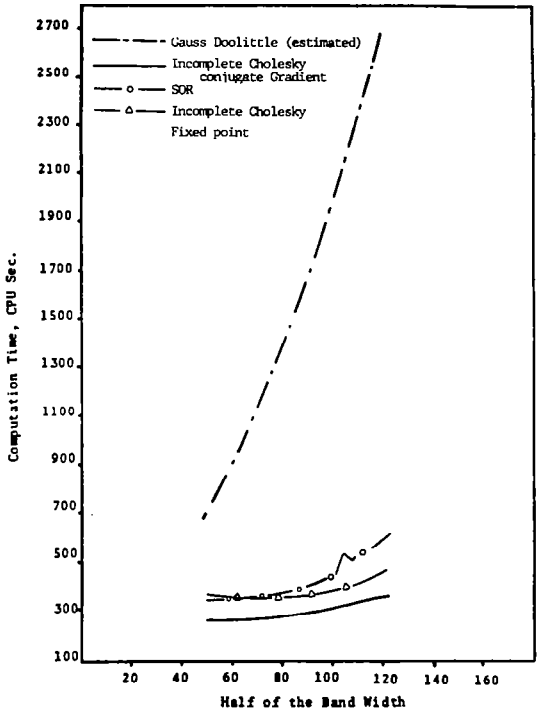

Figure 6.- Effect of Jacobian band width on total computation time for 1100 node cylinder models.