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*Element And time step Criteria for Solving Time -
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presented by

Reza Maadooliat

has been accepted towards fulfillment
of the requirements for

Ph.D degree in AE

Larry Segerlund
Major professor

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ELEMENT AND TIME STEP CRITERIA FOR
SOLVING TIME-DEPENDENT FIELD PROBLEMS
USING THE FINITE ELEMENT METHOD

by

Reza Maadooliat

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ABSTRACT

ELEMENT AND TIME STEP CRITERIA FOR SOLVING TIME-DEPENDENT FIELD PROBLEMS USING THE FINITE ELEMENT METHOD

By

Reza Maadooliat

The method of estimating an optimum integration time step for irregular finite element grids was established by use of subregion analysis. The lumped and consistent formulations, a study of element matrices relative to the concepts of Positive Coefficients Rule and the determination of which elements are the most suitable for use in time dependent field type problems were also investigated.

The matrix stability analysis and Dusenberre's Criteria were used to study solutions to $[C]\{\dot{\phi}\} + [K]\{\phi\} - \{F\} = \{0\}$. The matrices $[A]$ and $[P]$ in the finite difference solution in time, $\{\phi\}_1 = [A]^{-1}[P]\{\phi\}_0 + [A]^{-1}\{F\}$, must satisfy the following criteria in order to avoid numerical oscillations and ensure physical reality.

1. $[A]$ must have positive diagonal coefficients and negative off-diagonal coefficients.
2. $[P]$ must be positive definite and have positive coefficients.

Other conclusions of the study include: a) Quadratic elements can not satisfy the requirements placed on $[A]$ and their use will always result in physical unrealistic values

for some of the nodes; b) the interior angles of the linear triangular element must be less than or equal to 90° ; c) the aspect ratio for the bilinear rectangular element must be less than $\sqrt{2}$; d) dividing a rectangle into two triangular elements significantly reduces the allowable time step; e) the convection matrix must be lumped if the criteria on $[A]$ is to be satisfied for all values of the convection coefficient.

The maximum allowable integration time step for the consistent finite element formulations is small compared to the lumped formulations. The satisfaction of Positive Coefficients Rule is also very difficult if not impossible for consistent formulations. The maximum eigenvalue of a subregion consisting of the five smallest elements in a grid yields a good estimate for the integration time step.

Approved _____
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Dedicated to:
Susan, Sohila and Mehdi

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CHAPTER I

INTRODUCTION

An analytical solution of the heat conduction for mixed boundary conduction defined on irregular geometries is in general very difficult if not impossible to obtain. Many of the practical heat conduction problems have no known analytical solution.

The finite difference method and the finite element method have been used by many people to solve the heat conduction equation. The finite element scheme has received much recent attention because of its ease in handling irregular nodal point locations, and mixed boundary conditions. The unique aspects of finite element solution is the integral formulation and the associated approximation equation.

Applying a finite element scheme to the heat conduction equation or a similar equation reduces the partial differential equation (PDE) to a system of algebraic or differential equations. The solution of the system of differential equations is not simple and straightforward. Many solution schemes exist and there are difficulties associated with each scheme. Some of these problems are discussed in the following sections.

1.1 NUMERICAL OSCILLATIONS

The first problems are those of stability and numerical oscillations. This aspect of the numerical study has nothing to do with the original partial differential equation (PDE) but rather concerns the investigation of errors in the arithmetic operations needed to numerically solve a system of ordinary differential equations (ODE). Although, there is an analytical solution for the system of ODE's, the system is often solved using a numerical method. In this process, the ODE's are transformed into difference equations which have an error associated with their solution. The total error is the numerical error plus the discretization error.

The numerical error comes from rounding. According to Welty (1974), this error is negligible in modern computing machinery.

The discretization error originates from the replacement of an ordinary differential equation by a finite difference equation. This error may be reduced by reducing the size of integration time step (ITS).

The following three figures illustrate some of the situations associated with stability and numerical oscillations when calculating the temperature distribution in an insulated rod of unit length whose ends are kept at a constant temperature of zero. The initial temperature distribution is:

$$\begin{array}{ll}
 T=2X & 0 \leq X \leq 1/2 \\
 \text{and} & \\
 T=2(1-X) & 1/2 \leq X \leq 1
 \end{array} \tag{1.1}$$

Figure 1.1 illustrates a typical stable and convergent solution. Figure 1.2 is stable, but oscillates about the exact solution. Figure 1.3 shows an unstable finite difference scheme. The temperature values oscillate about the exact solution and become worse with increased time. The size of the integration time step is responsible for the numerical oscillation and the unstable solution.

The question at hand is, "How large can the time step be and still avoid the numerical oscillation?" The answer for some finite difference methods are available, Myers (1971), Yalamanchili (1973). The difficulty arises when the region of the body does not have a nice shape and is composed of several materials or has mixed boundary conditions. Finite element grids are nearly always irregular and little information for estimating the allowable time step for irregular grids is available. For example, the ANSYS finite element program manual Swanson (1981) suggest that the finite difference estimate for a uniform grid be used to estimate the integration time step. It is also pointed out that the presence of heat transfer mechanisms other than conduction, such as radiation, etc. may require additional guidelines for selecting ITS. For example, abrupt changes in the ITS (i.e., changes by more than a

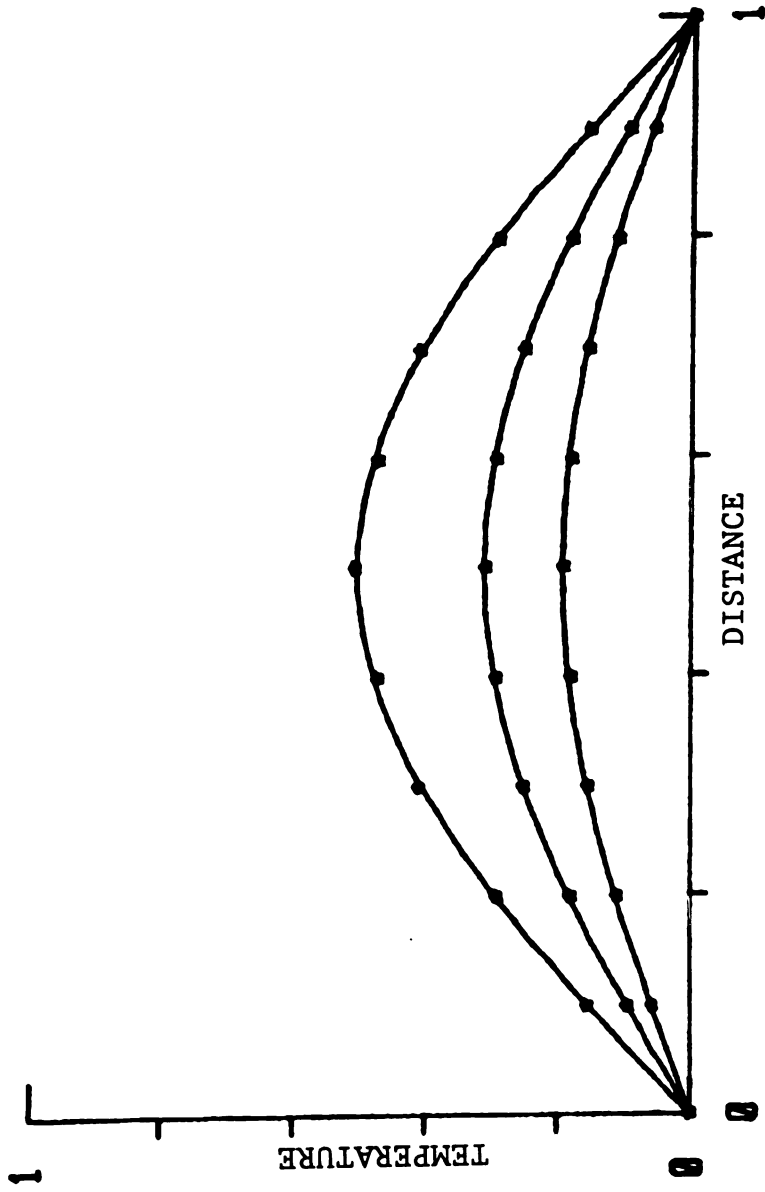


Figure 1.1 Stable convergent solution.

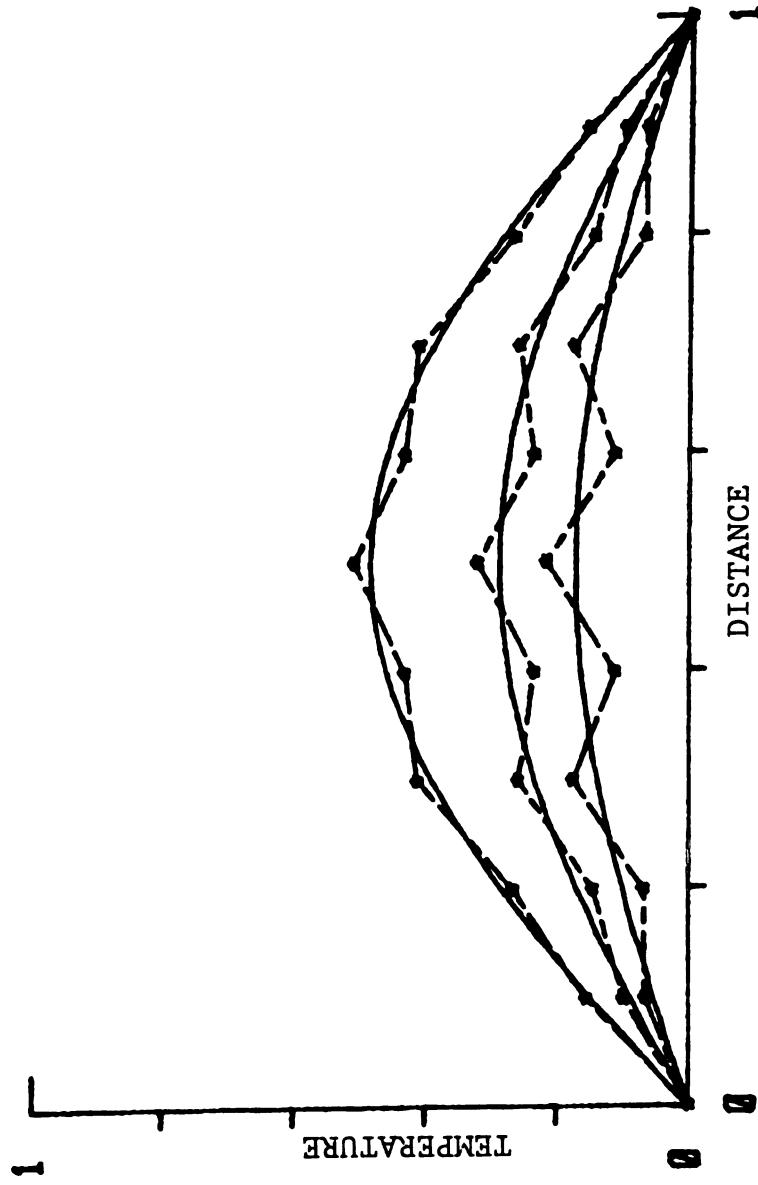


Figure 1.2 Stable and oscillating solution.

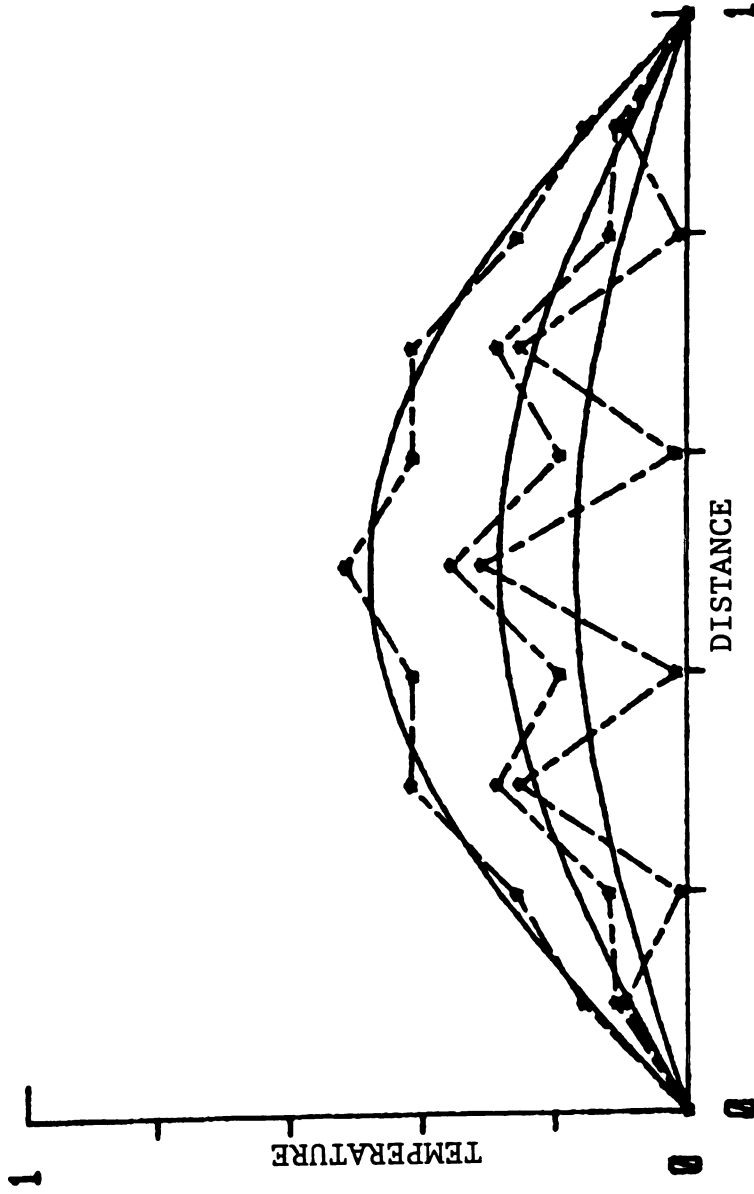


Figure 1.3 Unstable solution.

factor of 10) between consecutive load steps are not recommended unless the temperature change is fairly linear or constant.

The selection of the initial ITS for the ANSYS program is based on the properties of a single element and not on the entire grid. This criteria ignores the existence of elements of different sizes, composite materials and mixed boundary conditions.

The finite element program developed by Marc Analysis uses a percentage increase criteria when determining the time step (Segerlind, 1983). A time step value is specified and a set of temperatures at time $i+1$ are calculated. If any of the new values differ from their previous value by more than a specified percentage, the time step is reduced, the temperatures at time $i+1$ are discarded and a new set of values are calculated. This procedure is repeated for each time step until the percentage criteria is met.

1.2 CONSISTENCY AND CONVERGENCE

Another source of problems is the conversion from the PDE to the ODE's. In this case, the solution of the ordinary differential equation is not consistent with the PDE. This difficulty has nothing to do with the numerical integration. An analytical solution to the ODE even produces undesirable results. The analysis of consistency and convergence relative to the finite element method can be compared with this topic in finite difference analysis. Some

finite difference schemes, the Euler method for example, are conditionally convergent while the implicit approximations, such as Crank-Nicolson and the purely implicit method, are unconditionally convergent (Lapidus, 1982).

The idea of consistency may be clarified through an easy example. It is desired to calculate the temperature distribution in an insulated rod with a zero temperature distribution and heat input at the first node, Figure 1.4. Using linear elements and a consistent heat capacitance matrix, the numerical solution to the ODE shows that the temperature value for the second node is negative. This effect violates physical reality. This example is considered in detail in a later chapter.

1.3 OBJECTIVES

The selection of an allowable time step is important to making productive numerical computations. Some researchers based their selection of a time step criterion on a "worst case" guess like considering only element which requires the maximum ITS, Welty (1974). Others like Myers, (1977) based their criterion for the selection of time step on the Gerschgorin eigenvalue bound, which is a conservative estimate. One objective of this study is to develop a method of estimating an integration time step for irregular finite element grids.

Other objectives include a study of the lumped and consistent formulations, a study of element matrices

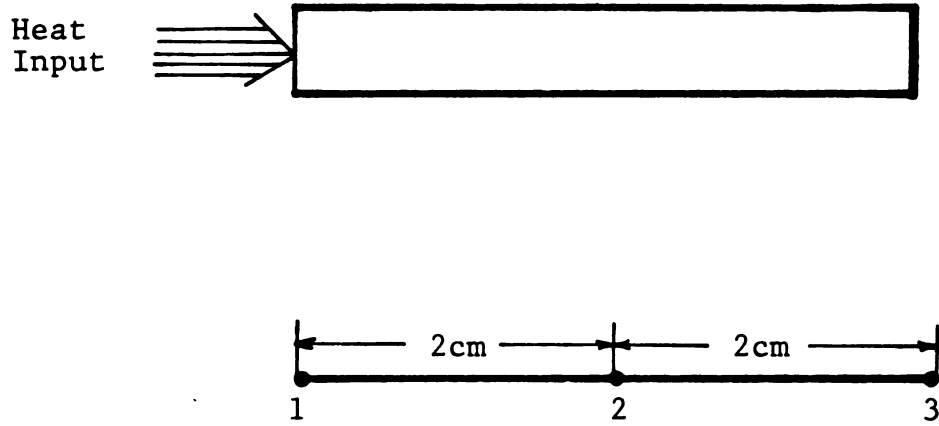


Figure 1.4 Heat transfer analysis in an insulated rod.

relative to the concepts of consistency and convergence and the determination of which elements are the most suitable for use in time dependent field type problems.

CHAPTER II

LITERATURE REVIEW

The time dependent field problem and its finite element formulation are reviewed in this chapter along with the stability and non-oscillation criteria for ordinary differential equations resulting from partial differential equations.

2.1 FUNDAMENTAL CONSIDERATIONS

The general form of Fourier's heat conduction in two-dimensions is

$$\rho C \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} (K_x \frac{\partial T}{\partial x}) + \frac{\partial}{\partial y} (K_y \frac{\partial T}{\partial y}) + Q \quad (2.1)$$

where K_x and K_y are thermal conductivities in the x and y directions respectively, ρ is the density, C is the specific heat and Q is a source term. Each of the parameters can be a function of position and temperature. The source term Q is positive if heat is put into the body. For an isotropic material, the general equation reduces to

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{Q}{K} = \frac{1}{\alpha} \frac{\partial T}{\partial t} \quad (2.2)$$

where $\alpha = K/\rho C$ is the thermal diffusivity. The transient period which occurs between the starting of the physical process and reaching the steady state condition (if it exists) is the period of interest in this study.

The region for (2.2) is shown in Figure 2.1. The shape is generally not a nice geometrical one. The boundary conditions are:

$$\text{Specified Temperature: } T = T_s \quad (2.3)$$

$$\text{Neumann conditions: } \frac{\partial T}{\partial n} = 0 \quad (2.4)$$

$$\text{Convectives: } K \frac{\partial T}{\partial n} = h(T - T_f) \quad (2.5)$$

where h is convective heat transfer coefficient, T_f is the ambient temperature and n is the outward normal to the boundary. The parameters h , T_f and T_s are assumed time and temperature independent but can vary with the position on the boundary. The initial condition is

$$T(x, y, 0) = T_0(x, y) \quad (2.6)$$

The finite-difference formulation is obtained by replacing the derivatives in the PDE by difference equations. In the finite element technique, the variational statement of the problem is used to obtain the system of differential equations. The functional formulation that is equivalent to (2.1) is, Segerlind (1976),

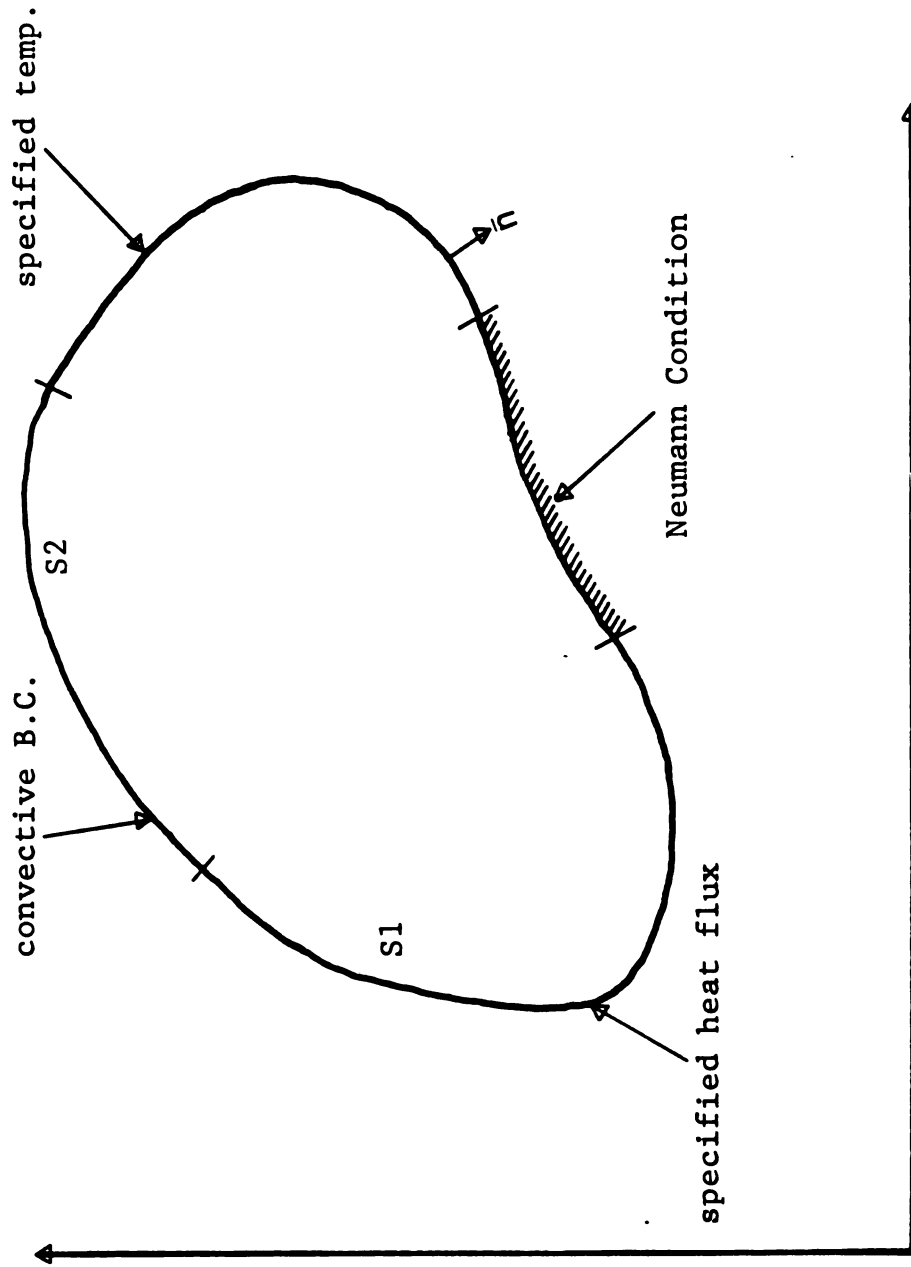


Figure 2.1 General two-dimensional heat conduction problem.

$$\begin{aligned}
\pi = & \int_V 1/2 \left[K_x \left(\frac{\partial T}{\partial x} \right)^2 + K_y \left(\frac{\partial T}{\partial y} \right)^2 - 2(Q - \rho C \frac{\partial T}{\partial t})T \right] dv \\
& + \int_{s_1} q T ds + \int_{s_2} \frac{h}{2} (T - T_f)^2 ds
\end{aligned} \tag{2.7}$$

where T_f is the ambient temperature, V is the volume of the body, and S is the surface area. Defining two matrices

$$\{g\}^T = \begin{bmatrix} \frac{\partial T}{\partial x} & \frac{\partial T}{\partial y} \end{bmatrix} \tag{2.8}$$

and

$$[D] = \begin{bmatrix} K_x & 0 \\ 0 & K_y \end{bmatrix} \tag{2.9}$$

(2.7) can be written as

$$\begin{aligned}
\pi = & \int_V 1/2 \left[\{g\}^T [D] \{g\} - (Q - \rho C \frac{\partial T}{\partial t})T \right] dv \\
& + \int_{s_1} q T ds + \int_{s_2} \frac{h}{2} (T - T_f)^2 ds
\end{aligned} \tag{2.10}$$

The function for T is continuous but defined by several equations over the region. The individual equations, $T^{(e)}$, are defined over subregions called elements and the above equation should be separated into integrals over the individual elements, therefore,

$$\begin{aligned}
\pi = & \sum_{e=1}^E \int_{V(e)}^{1/2} \left[\{g^{(e)}\}^T [D] \{g^{(e)}\} \right] dv \\
& - \int_{V(e)} T^{(e)} \left[Q^{(e)} - \rho^{(e)} c^{(e)} \frac{\partial T^{(e)}}{\partial t} \right] dv \\
& + \int_{s_1(e)} T^{(e)} q^{(e)} ds + \int_{s_2(e)} \frac{h^{(e)}}{2} (T^{(e)} - T_f)^2 ds
\end{aligned} \tag{2.11}$$

or

$$\pi = \sum_{e=1}^E \pi^{(e)}$$

where E is the total number of elements. The function π is minimized with respect to a set of nodal values contained in $\{T\}$. Minimization produces

$$\frac{\partial \pi}{\partial \{T\}} = \frac{\partial}{\partial \{T\}} \sum_{e=1}^E \pi^{(e)} = \sum_{e=1}^E \frac{\partial \pi^{(e)}}{\partial \{T\}} = 0 \tag{2.13}$$

The temperature in each element is given by

$$T^{(e)} = N_i^{(e)} T_i + N_j^{(e)} T_j + \dots + N_m^{(e)} T_m \tag{2.14}$$

or

$$T^{(e)} = [N^{(e)}] \{T^{(e)}\} \tag{2.15}$$

where $[N^{(e)}]$ is a row vector of shape functions (interpolation functions) and $\{T^{(e)}\}$ are element nodal temperatures $\{T^{(e)}\}^T = [T_i \ T_j \ \dots T_m]$.

Some properties of the interpolating functions include:

1. The interpolating functions must sum to one at every point in the element.

$$N_i + N_j + \dots + N_m = 1$$

2. The derivative of the shape functions with respect to a variable sums to zero, i.e.,

$$\frac{\partial N_i}{\partial x} + \frac{\partial N_j}{\partial x} + \dots + \frac{\partial N_m}{\partial x} = \frac{\partial}{\partial x}(N_i + N_j + \dots + N_m) = \frac{\partial}{\partial x}(1) = 0 \quad (2.16)$$

The temperature gradient can be written in terms of the interpolation functions as

$$\{g^{(e)}\} = [B^{(e)}] \{T^{(e)}\} \quad (2.17)$$

where $[B^{(e)}]$ is a gradient matrix

$$[B] = \begin{bmatrix} \frac{\partial N_i}{\partial x} & \frac{\partial N_j}{\partial x} & \dots & \frac{\partial N_m}{\partial x} \\ \frac{\partial N_i}{\partial y} & \frac{\partial N_j}{\partial y} & \dots & \frac{\partial N_m}{\partial y} \end{bmatrix}$$

Introducing (2.14) and (2.17) into the functional and performing the minimization, gives the matrix differential equations, Segerlind (1976).

$$[C]\frac{\partial \{T\}}{\partial t} + [K]\{T\} = \{F\} \quad (2.19)$$

where the element contributions to $[C]$, $[K]$ and $\{F\}$ are the element capacitance matrix

$$[C^{(e)}] = \int_V \rho c [N]^T [N] dv \quad (2.20a)$$

The element stiffness matrix

$$[k^{(e)}] = \int_V [B]^T [D] [B] dv + \int_{s_2} h [N]^T [N] ds \quad (2.20b)$$

and the element force vector

$$\{f^{(e)}\} = - \int_V Q [N]^T dv + \int_{s_1} q [N]^T ds - \int_{s_2} h T_f [N]^T ds \quad (2.20c)$$

The three integrals are evaluated over each element and the element contributions are added using the direct stiffness procedure. A superscript (e) on the left of the equal sign implies that all the quantities on the right hand side are to be interpreted on an element basis.

2.2 SOME PROPERTIES OF $[k^{(e)}]$ AND $[c^{(e)}]$ MATRICES

The stiffness matrix (conductivity matrix), $[K]$, and the heat capacitance matrix, $[C]$, have some interesting properties.

1. Writing (2.20b) using indicial notation and deleting the surface integral, which means either no losses through boundaries or a specified boundary temperature, a coefficient in the element matrix is

$$k_{i,j} = \int_V K_x \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} dx + \int_V K_y \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} dy \quad (2.21)$$

Taking the sum of the i^{th} row of $[k^{(e)}]$

$$\begin{aligned} \sum_{j=1}^{NP} k_{i,j} &= \text{sum of individual coefficients in } i^{\text{th}} \text{ row} \\ &= \int_V K_x \frac{\partial N_i}{\partial x} \left(\sum_{j=1}^{NP} \frac{\partial N_j}{\partial x} \right) dv + \int_V K_y \frac{\partial N_i}{\partial y} \left(\sum_{j=1}^{NP} \frac{\partial N_j}{\partial y} \right) dv \\ &= 0 \end{aligned} \quad (2.22)$$

because of (2.16).

2. Because the derivatives with respect to x or y sum to zero, it is easy to verify that $[K]$ is singular. The last column of $[K]$ is a linear combination of the previous columns because of property one, i.e., the i^{th} row of the matrix has the following property.

$$k_{i,1} + k_{i,2} + \dots + k_{i,m} = 0 \quad (2.23)$$

or

$$k_{i,m} = -(k_{i,1} + k_{i,2} + \dots + k_{i,m-1}) \quad (2.24)$$

3. The global matrix $[K]$ is symmetric and sparse, Segerlind (1976). This property is particularly important in reducing the computer storage for efficient computations.

4. The capacitance matrix $[C]$ is a positive definite matrix while $[K]$ is semi-definite. If the surface integral in (2.20b) is included, $[K]$ is positive definite Fried, (1979).

2.3 MODAL ANALYSIS

The technique of modal analysis is the discrete counterpart to the separation of variables and has the property of uncoupling the system of ODE in (2.19). The method is based on the expression of the nodal temperatures as a linear combination of the orthonormal eigenvectors of the global system $[K]\{X\} = \lambda[C]\{X\}$. The temperature values can be written as

$$\{T\} = \sum_{j=1}^N \alpha_j(t) \{x_j\} \quad (2.25)$$

and

$$\{\dot{T}\} = \sum_{j=1}^N \dot{\alpha}_j(t) \{x_j\} \quad (2.26)$$

where $\alpha_j(t)$ are time dependent coefficients and $\{X_j\}$ are orthonormal eigenvectors of the form $[K]\{X\} = \lambda[C]\{X\}$.

Introducing (2.25) and (2.26) into (2.19)

$$\{T\} = \sum_{j=1}^N \alpha_j [K]\{X_j\} + \sum_{j=1}^N \alpha_j [C]\{X_j\} = \{f(t)\} \quad (2.27)$$

or with

$$[K]\{X_j\} = \lambda_j [C]\{X_j\}$$

$$\sum_{j=1}^N (\lambda_j \alpha_j + \dot{\alpha}_j) [C]\{x_j\} = \{f(t)\} \quad (2.28)$$

Since $[C]$ and the eigenvectors $\{X\}$ form an orthonormal system, Eq. (2.28) may be decoupled by premultiplying it by $\{X_1\}^T, \{X_2\}^T, \dots, \{X_N\}^T$.

$$\lambda_j \alpha_j + \dot{\alpha}_j = \{X_j\}^T \{f(t)\} \quad (2.29)$$

This generates N equations; each one is solved separately for α_j . The initial value of α_j can be computed from Eq. (2.25).

$$\alpha_j(0) = \{X_j\}^T \{T(0)\} \quad (2.30)$$

where $\{T(0)\}$ is the initial nodal temperature distribution.

For a large system of differential equations, the requirement that all eigenvalues and eigenvectors be known makes the modal analysis computations very expensive and impractical. Therefore, a finite difference numerical solution in time has been used as a means of solving (2.19).

2.4 DIFFERENCE RECURRENCE FORMULA

The system of first-order linear differential equations, (2.19), and the vector of initial values (2.6), define the transient heat conduction problem. Modal analysis and a similar method suggested by Myers (1977) are exact solutions to the differential system (2.19), but these methods are so complicated for large systems that they are seldom used. The usual solution procedure is to integrate the system of differential equations with the aid of digital computer. The most crucial step is choosing a method of integration which is accurate and efficient.

The general method for obtaining a numerical solution to the differential equations given by (2.19) is based on the finite difference approximation in the time domain. The procedure moves ahead in time according to the relation

$$\{T\}_{n+1} = \{T\}_n + [(1-\theta)\{\dot{T}\}_n + \{\dot{T}\}_{n+1}]\Delta t \quad (2.31)$$

where n represents the time step index and Δt is the time interval. The time difference parameter, θ , gives a weighted average time derivative over the time interval Δt .

In applying (2.31) to the finite element problem, pre-multiply it by $[C]$ and then use (2.19) to eliminate the time derivatives. The result is

$$[C]\{T\}_{n+1} = [C]\{T\}_n + [C]\left((1-\theta)\{\dot{T}\}_n + \theta\{\dot{T}\}_{n+1}\right)\Delta t \quad (2.32)$$

or

$$\begin{aligned} ([C] + \theta\Delta t[K])\{T\}_{n+1} = & ([C] - (1-\theta)\Delta t[K])\{T\}_n \\ & + \Delta t(1-\theta)\{F\}_n + \theta\Delta t\{F\}_{n+1} \end{aligned} \quad (2.33)$$

Eq. (2.33) gives the new temperature, $\{T\}_{n+1}$ in terms of a set of known values. The $\{T\}_n$ is known from earlier computations (or from initial conditions for the first step). The time difference parameter, θ , as well as force vectors, $\{F\}_n$ and $\{F\}_{n+1}$, must be specified. There are four popular choices for θ . These choices and their associated names are, Segerlind (1976).

- a) $\theta = 0$ Forward Difference Method (Euler's Method)
- b) $\theta = 1/2$ Central Difference Method (Crank-Nicolson Method)
- c) $\theta = 2/3$ Galerkins Difference Method
- d) $\theta = 1$ Backward Difference Method

The finite difference equation for any value of θ , can be written in a general form

$$[A]\{T\}_{n+1} = [P]\{T\}_n + \{F^*\} \quad (2.34)$$

where $[A]$ and $[P]$ are combinations of $[C]$ and $[K]$ and are dependent on the material properties and the time step Δt . Also, the vector $\{F^*\}$ in (2.34) is a combination of $\{F\}_n$ and $\{F\}_{n+1}$. These matrices are shown in Table 2.1 for different cases:

Table 2.1:

$[A]$ and $[P]$ for the popular choices of θ

Method	$[A]$	$[P]$
$\theta = 0$	$[C]$	$[C] - \Delta t[K]$
$\theta = 1/2$	$[C] + (\Delta t/2)[K]$	$[C] - (\Delta t/2)[K]$
$\theta = 2/3$	$[C] + (2\Delta t/3)[K]$	$[C] - (\Delta t/3)[K]$
$\theta = 1$	$[C] + \Delta t[K]$	$[C]$

2.5 PROPERTY OF $[A]^{-1}[P]$ MATRIX

When the governing differential equation, (2.1), contains only the derivative of the temperature variable, the vectors $\{T\}$ and $\{T+C\}$ (where C is a constant vector) both satisfy the differential equation. This property must also be reflected by the difference equation (2.34), therefore,

$$\{T+C\}_{n+1} = [A]^{-1}[P] \{T+C\}_n \quad (2.35)$$

which requires the sum of each row in $[A]^{-1}[P]$ be unity. This fact can be shown for the case when the system has

insulated boundary condition with a heat source input ($[K]$ is singular). In this situation, the unity vector $\{u\}^T$, $[1,1,\dots,1]$, is the eigenvector of $[A]^{-1}[P]$ with an eigenvalue of one which is the requirement for sum of the rows in a matrix be unity.

$$[A]^{-1}[P]\{u\} = \{u\} \quad (2.36)$$

Upon multiplying by $[A]$

$$[P]\{u\} = [A]\{u\} \quad (2.37)$$

or from Table 2.1

$$([C] - \Delta t(1 - \theta)[K])\{u\} = ([C] + \Delta t\theta[K])\{u\} \quad (2.38)$$

Writing the i^{th} equation of (2.38) we obtain

$$\sum_{j=1}^N C_{i,j} - \Delta t(1-\theta)k_{i,j} = \sum_{j=1}^N C_{i,j} + (\theta\Delta t)k_{i,j} \quad (2.39)$$

From which the above equation requires that

$$\sum_{j=1}^N k_{i,j} = 0 \quad (2.40)$$

Since (2.40) holds for these cases, the Eq. (2.35) is true.

2.6 STABILITY AND OSCILLATION ANALYSIS

The concepts of stability and numerical oscillations for the general matrix difference equation (2.34) are introduced in this section.

The numerical solution of equation (2.34) has nothing to do with the PDE but rather is concerned with the boundedness of all errors in the arithmetic operations needed to solve the system of difference equations. The effort required to calculate nodal temperatures for a given amount of time increases greatly for small time intervals, therefore, it is desirable to choose the time intervals as large as possible. The allowable size of the interval is a part of stability analysis.

There are several ways of defining a stability criteria. The most popular ones are a general approach, Heuristic Stability, Von-Neumann's Method, and matrix stability.

2.6.1 General Approaches

A general approach to defining stability and oscillation criterion is obtained by using the method of separation of variables and the prescribed boundary conditions. The resulting solution is used to establish the stability requirements. The full details of the technique for one dimensional field problems can be seen in Lemmon (1969) and for two dimensional field problems in Yalamanchili

(1973). This method is not discussed in detail here because it is applicable only to uniform grids.

2.6.2 Heuristic Stability

The Heuristic approach to stability introduces a single error at one nodal point and investigates the amount of error in each time step. If the error dampens out, the system of difference equations is stable, otherwise it is unstable. The approach yields no information, unless an effort is made to determine possible bounds on the stability. Details and illustration of the procedure can be found in Lapidus (1982).

2.6.3 Von Neumann's Method

Von Neumann's method for stability analysis which was developed for continuous systems, has been modified for use with matrix equations. A full explanation of the method can be found in O'Brien et al. (1951). A partial discussion goes as follows.

Eq. (2.34) can be solved for the new temperatures $\{T\}_{n+1}$ giving

$$\{T\}_{n+1} = [A]^{-1}[P]\{T\}_n + [A]^{-1}\{F^*\} \quad (2.41)$$

The matrix $[A]$ is assumed to be non-singular. The error, due to round off, must satisfy the following homogeneous equation, Leech (1965).

$$\{e_r\}_{n+1} = [A]^{-1}[P]\{e_r\}_n \quad (2.42)$$

Let the error be given by

$$\{e_r\}_n = e^{n\alpha\Delta t}\{\delta\} \quad (2.43)$$

where $\{\delta\}$ is an arbitrary vector. Combining (2.42) and (2.43) gives

$$e^{\alpha\Delta t}\{\delta\} = [A]^{-1}[P]\{\delta\} \quad (2.44)$$

for $e^{\alpha\Delta t} = \mu$, (2.44) yields

$$[A]^{-1}[P]\{\delta\} = \mu\{\delta\} \quad (2.45)$$

and the μ 's are the standard eigenvalue associated to the matrix $[A]^{-1}[P]$. Since, $[A]$ and $[P]$ are symmetric with real coefficients each μ is real. The general expression for the error is

$$\{e_r\}_n = \mu^n\{\delta\} \quad (2.46)$$

The stability criterion is obtained from the final error equation which says the error should be bounded with respect to time. For stability requirements, the magnitude of μ must be less than or equal to one.

$$|\mu| \leq 1 \quad (2.47)$$

To avoid numerical oscillations the quantity μ must be bounded between zero and one.

$$0 < \mu < 1 \quad (2.48)$$

It is worthwhile to remember that the standard eigenvalue problem given by (2.45) can be written as a general eigenvalue problem.

$$[P]\{\delta\} = \mu[A]\{\delta\} \quad (2.49)$$

This form and the general eigenvalue problem of

$$[K]\{x\} = \lambda[C]\{x\}$$

are used later to obtain stability requirements for the system of difference equations (2.34).

2.6.4 Dusinberre Concepts

The analysis of stability from physical considerations has been developed by several people including Dusinberre (1961) and Patankar, (1980). It is easy to think of an equation in (2.41) as having the form

$$T_p = \sum_{n=1}^r a_{pn} T_n + f_p \quad (2.50)$$

where a_{pn} is a coefficient in $[A]^{-1}[P]$, f_p the coefficient in $[A]^{-1}\{F^*\}$, T_p the temperature at any nodal point in the region influenced by the values of r nodal points. An increase in the temperature of a node, other than node p , while maintaining the rest of the nodes at their same temperature (excluding node p) means that the temperature T_p

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must increase. This idea leads to the fact that the neighboring coefficient must be positive. A simple rule is "avoid negative coefficients in any row of $[A]^{-1}[P]$. Also, using a similar argument, the coefficients in $[A]$ to be positive. This criteria is used when analyzing the elements in future chapters.

2.6.5 Matrix Stability

The matrix approach to stability analysis is illustrated using the scheme known as Euler's method. The force vector in a matrix differential (or difference) equation has no role in the stability investigation Trujillo (1977). This fact can be seen in the final form of the difference equation for the temperature formula (2.41). Eq. (2.41) can be written in the form

$$\{T\}_n = ([A]^{-1}[P])^n \{T\}_0 + [A]^{-1}[P]^{n-1} \{F^*\} + \dots + \{F^*\} \quad (2.51)$$

which allows for an easier analysis. The term $([A]^{-1}[P])^n$ alone in (2.51) is sufficient for stability investigations. The remaining terms in the right hand side of the equation are stable as long as $[A]^{-1}[P]$ is stable.

For matrix differential equations, usually the method of a variational parameter is used to solve the system of linear ODE. The influence of the forcing term is reflected in the variable coefficients of the solution related to the homogeneous part. Therefore, the analysis can be done using a differential equation with the right hand side zero

i.e.,

$$[C]\{\dot{T}\} + [K]\{T\} = 0 \quad (2.52)$$

with initial conditions

$$T(0) = T_0 \quad (2.53)$$

Euler's method has the form

$$[C]\{T\}_{n+1} = ([C] - \Delta t[K]) \{T\}_n \quad (2.54)$$

Multiplying through by $[C]^{-1}$ and writing the temperature distribution in terms of initial temperature values, yields

$$\{T\}_n = ([I] - \Delta t[C]^{-1}[K])^n \{T\}_0 \quad (2.55)$$

The initial temperatures, $\{T\}_0$, is expanded in terms of the eigenvectors $\{X_1\}, \{X_2\}, \dots, \{X_n\}$ of $[K]\{X\} = \lambda[C]\{X\}$ to give

$$\begin{aligned} \{T\}_n &= ([I] - \Delta t[C]^{-1}[K])^n \{T\}_0 \\ &= ([I] - \Delta t[C]^{-1}[K])^n (C_1\{X_1\} + C_2\{X_2\} + \dots C_N\{X_N\}) \end{aligned}$$

Consider the following calculations

$$\begin{aligned}
([I] - \Delta t[C]^{-1}[K])\{X_j\} &= \{X_j\} - \Delta t[C]^{-1}[K]\{x_j\} \\
&= \{X_j\} - \Delta t[C]^{-1}\lambda_j[C]\{X_j\} \\
&= \{X_j\} - \Delta t\lambda_j\{X_j\} \\
&= (1 - \Delta t\lambda_j)\{x_j\}
\end{aligned} \tag{2.57}$$

Therefore,

$$\begin{aligned}
([I] - \Delta t[C]^{-1}[K])^n\{X_j\} &= ([I] - \Delta t[C]^{-1}[K])^{n-1}(1 - \Delta t\lambda_j)\{X_j\} \\
&= (1 - \Delta t\lambda_j)^n\{X_j\}
\end{aligned} \tag{2.58}$$

or

$$\{T\}_n = C_1(1 - \lambda_1\Delta t)^n\{X_1\} + C_2(1 - \lambda_2\Delta t)^n\{X_2\} + \dots + C_n(1 - \lambda_N\Delta t)^n\{X_N\} \tag{2.59}$$

For this system to be stable the quantity in each parenthesis must be less than or equal to one. All of the eigenvalues of $[C]$ and $[K]$ are positive and real thus only the largest value of λ needs to be considered. This consideration gives

$$-1 < 1 - \lambda_N\Delta t \quad \text{or} \quad \Delta t < 2/\lambda_N \tag{2.60}$$

where λ_N is the largest eigenvalue of $[K]\{X\} = \lambda[C]\{X\}$. The computation of λ_N is relatively easy but none of the commercial finite element programs do this relative to a time dependent field problem.

2.7 STABILITY CRITERION FOR GENERAL SCHEME

The maximum allowable time step for Euler's method is known as a critical time step, Meyer (1977). It is denoted by Δt_c and is a device to study the character of the approximate solution relative to the oscillation or non-oscillation of the calculated values. The stability limit of (2.60) was obtained for a simple explicit scheme (Euler's method), but it can be extended to the other important cases such as the central difference method $\theta = 1/2$, and Galerkin's method, $\theta = 2/3$.

The stability limit requires that the magnitude of the eigenvalues of $[A]^{-1}[P]$ matrix, λ_θ , be less or equal to one. The relation between λ_θ and λ has been established by Meyers, (1977). The eigenvalue of $[A]^{-1}[P]$ are determined from the relation

$$\det([A]^{-1}[P] - \lambda_\theta [I]) = 0 \quad (2.61)$$

This equation can be multiplied by $\det[A]$ to get

$$\det[A]\det([A]^{-1}[P] - \lambda_\theta [I]) = 0$$

Since the product of the determinants of two matrices is equal to the determinant of the product of matrices, the above equation can be written as

$$\det([P] - \lambda_\theta [A]) = 0 \quad (2.62)$$

Substituting for [A] and [P] from Table 2.1, yields

$$\det([C] - (1 - \theta)\Delta t[K] - \lambda_{\theta}([C] + \theta\Delta t[K])) = 0$$

or (2.63)

$$\det\left([K] - \frac{1 - \lambda_{\theta}}{(1 - \theta + \theta\lambda_{\theta})\Delta t}[C]\right) = 0$$

Comparing the general eigenvalue problem of $[K]\{X\} = \lambda[C]\{X\}$ with (2.63) gives

$$\lambda_{\theta} = \frac{1 - \lambda(1 - \theta)\Delta t}{1 + \theta\lambda\Delta t} \quad (2.64)$$

Therefore, the stability limit of (2.41) is

$$\Delta t = 2/(1 - 2\theta)\lambda_N \quad (2.65)$$

and the non-oscillatory limit of (2.41) is

$$\Delta t = 1/(1 - \theta)\lambda_N \quad (2.66)$$

The variation of λ_{θ} with respect to $\psi = \lambda\Delta t$, for different values of θ is shown in Figure 2.2. It can be shown that for small time step all four schemes are identical. The solution begin to differ as the time step increases. The Crank-Nicolson scheme is always stable and the pure implicit method has only steady decay solution. The Euler's method is unstable for $\psi > 2$.

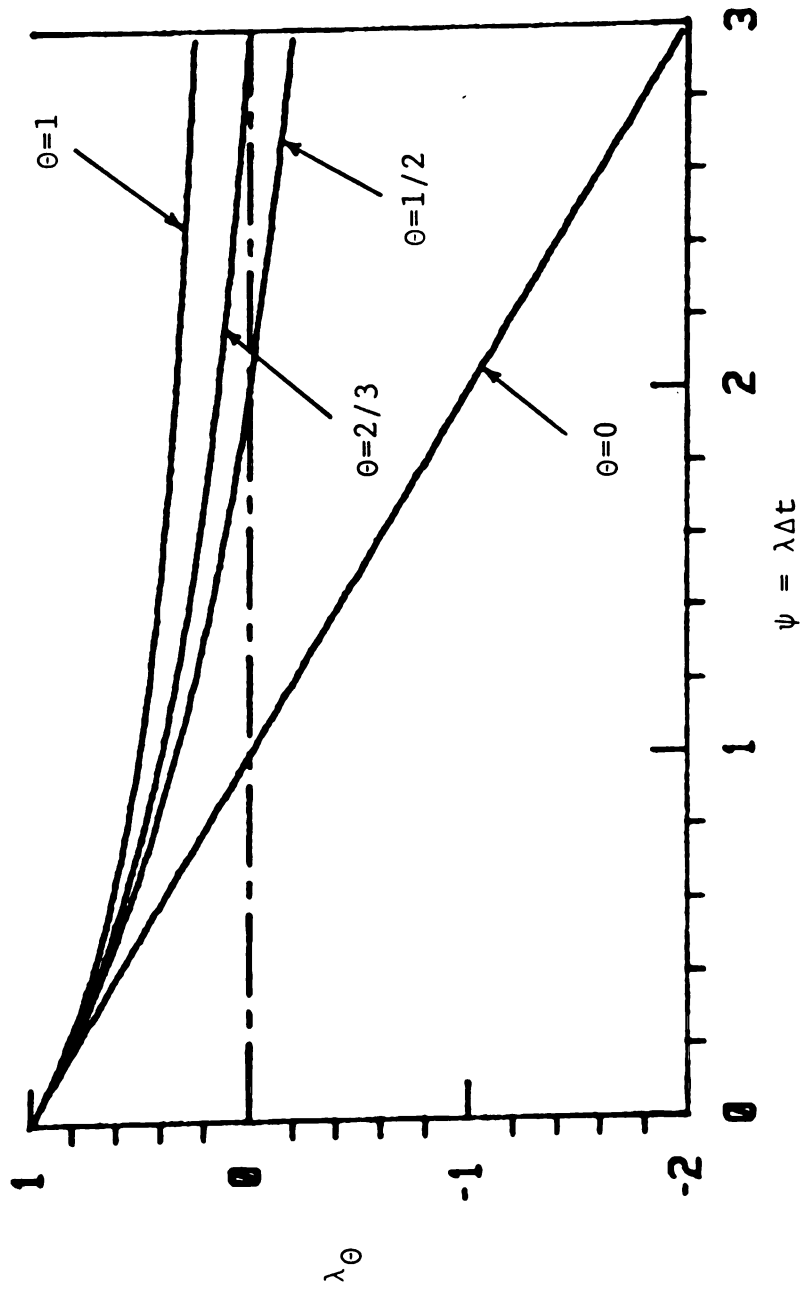


Figure 2.2 Variation of λ_θ with respect to ψ for different values of θ .

CHAPTER III

EVALUATION CRITERIA

As mentioned previously, the analysis of the time dependent heat conduction equation may be regarded as consisting of three parts: (i) Discretization process, (ii) numerical stability, and (iii) Dusenberre's concepts. The various kinds of stability analysis and the discretization concepts were discussed in the previous chapter. In this chapter the matrix stability along with the requirements of Dusenberre's criteria are explained.

3.1 MATRIX STABILITY

The non-oscillation criterion of equation (2.51) requires that the eigenvalue of $[A]^{-1}[P]$ matrix, λ_{θ} , to be bounded between zero and one. The eigenvalues, λ_{θ} , are all positive if the matrix $[P]$ remains positive definite.

From Eq. (2.64) the eigenvalue, λ_{θ} , is always less than one provided $[P]$ remains positive definite. Therefore, the non-oscillation criterion reduces to finding the minimum value of Δt that makes the matrix

$$[P] = [C] - (1-\theta)\Delta t[K]$$

singular. As a result, the analysis boils down to finding

the smallest eigenvalue of the equation

$$[C]\{X\} = a[K]\{X\} \quad (3.1)$$

where $a = (1 - \theta)\Delta t$. Consequently, the allowable time step should satisfy the following inequality

$$\Delta t \leq a/(1 - \theta) \quad (3.2)$$

which is exactly the same as Eq. (2.66), ($\lambda_N = 1/a$).

3.2 DUSINBERRE CONCEPT

The positive coefficients rule, discussed earlier, considers the stability criteria from the physical point of view. The coefficients a_{pn} , in (2.50), which come from $[A]^{-1}[P]$ have to be non-negative as well as the elements in $[A]^{-1}$.

One way to guarantee that the positive coefficients rule is satisfied is to require negative off-diagonal terms in matrix $[A]$ and positive coefficients in matrix $[P]$. This statement is based on the following analysis.

Knowing that every symmetric positive definite matrix has a unique Choleski Decomposition, the matrix $[A]$ can be decomposed into the product of a lower and an upper triangular matrix.

$$[A] = [L][L]^T \quad (3.3)$$

or

$$\begin{bmatrix} a_{11} & a_{12} \cdots a_{1n} \\ a_{21} & a_{22} \cdots a_{2n} \\ \vdots & \vdots \\ a_{n1} & a_{n2} \cdots a_{nn} \end{bmatrix} = \begin{bmatrix} l_{11} & & 0 \\ l_{21} & l_{22} & \\ \vdots & \vdots & \ddots \\ l_{n1} & l_{n2} \cdots l_{nn} \end{bmatrix} \begin{bmatrix} l_{11} & l_{21} \cdots l_{n1} \\ & l_{22} \cdots l_{n2} \\ & & \ddots \\ 0 & & & l_{nn} \end{bmatrix}$$

Using the general formula for Choleski factorization,

$$\left. \begin{aligned} l_{ii} &= \left(a_{ii} - \sum_{k=1}^{i-1} l_{ik}^2 \right)^{\frac{1}{2}} \\ l_{ij} &= \frac{a_{ij} - \sum_{k=1}^{j-1} l_{ik} l_{jk}}{l_{jj}} \end{aligned} \right\} \quad (3.4)$$

Jenning, (1977). It can be shown by induction that every diagonal of [L] is positive and all off-diagonal coefficients are negative. Also, the inverse matrix of [L] is a lower triangular matrix with all positive coefficients. As a result, the [A] matrix which is equal to $[L^{-1}]^T [L]^{-1}$ has positive coefficients.

3.3 EVALUATION CRITERIA

The evaluation criteria used in this study are:

1. The coefficients of $[A^{-1}][P]$ and $[A]^{-1}$ must be positive thus [A] must have positive diagonals and negative off-diagonal coefficients and [P] must have positive coefficients.

2. The matrix [P] must be singular or positive definite.

CHAPTER IV

CONSISTENT AND LUMPED FORMULATIONS

This chapter concerned with the consistent and lumped heat capacitance matrices. The usual finite element method produces a non-diagonal heat capacity matrix often called the consistent formulation. The diagonalization of the heat capacity matrix, however, has been considered by several researchers. The first to lump $[C]$ were Nickel and Wilson (1966).

The diagonalization of $[C]$ can be done by simply adding the coefficients in each row and placing the sum on the diagonal, Myers (1977). Some special numerical integrations also, have been suggested for making $[C]$ diagonal, Zienkiewicz (1977).

The lumped formulations reduces the computer storage requirements and the number of computations in the step-by-step solution. Users experience has shown that a larger allowable time step may be used before introducing the oscillations in the solutions.

The objective of this chapter is to compare the analytical and numerical solutions of the two methods and determine the operating region for the numerical solution of each procedure.

4.1 HEAT FLOW IN A ROD

This section compares the analytical solutions for the consistent and lumped formulations using the temperature distribution in an insulated rod, Figure 4.1, as an example. Heat input occurs at the left end and the right end is insulated. The initial temperature is zero.

The element matrices are given by

$$[k^{(e)}] = \begin{bmatrix} 2 & -2 \\ -2 & 2 \end{bmatrix}; \quad \text{and} \quad [C^{(e)}] = \begin{bmatrix} 8 & 4 \\ 4 & 8 \end{bmatrix}$$

The global matrices for two uniform elements are

$$[K] = \begin{bmatrix} 2 & -2 & 0 \\ -2 & 4 & -2 \\ 0 & -2 & 2 \end{bmatrix} \quad \text{and} \quad [C] = \begin{bmatrix} 8 & 4 & 0 \\ 4 & 16 & 4 \\ 0 & 4 & 8 \end{bmatrix}$$

and the forcing term is

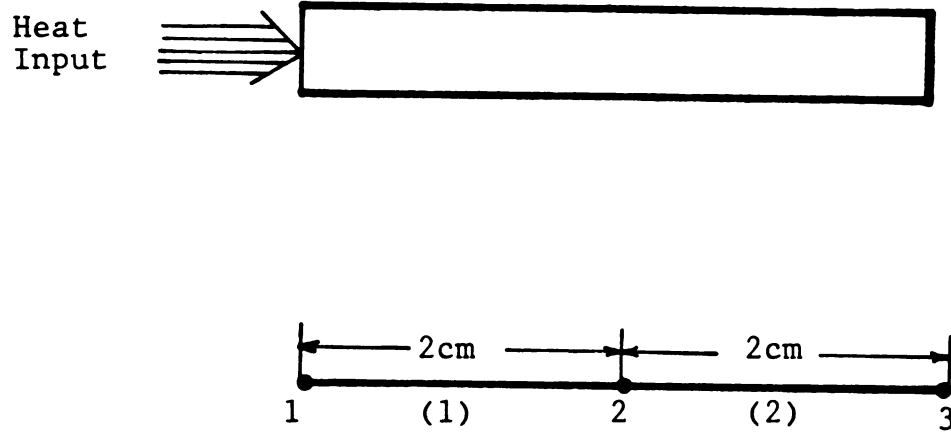
$$\{F\}^T = [5 \ 0 \ 0]$$

since the heat input is a point source.

4.1.1 Consistent Formulation

Substitution of $[K]$ and $[C]$ into (2.34) yields

$$\begin{bmatrix} 8 & 4 & 0 \\ 4 & 16 & 4 \\ 0 & 4 & 8 \end{bmatrix} \{\dot{T}\} + \begin{bmatrix} 2 & -2 & 0 \\ -2 & 4 & -2 \\ 0 & -2 & 2 \end{bmatrix} \{T\} = \begin{Bmatrix} 5 \\ 0 \\ 0 \end{Bmatrix} \quad (4.1)$$



$$K_x = \frac{4 \text{ watts} \cdot \text{cm}}{\text{C}^\circ}$$

$$P_c = 12 \frac{\text{watts}}{\text{sec} \cdot \text{cm} \cdot \text{C}^\circ}$$

$$A = 1 \text{ cm}^2$$

Figure 4.1 Insulated rod with heat at node 1.

The Laplace transform method is used to obtain the exact solution to the system of ordinary differential equations in (4.1). This method gives

$$CST(s) + KT(S) = F(s)$$

$$\text{or} \quad (4.2)$$

$$T(S) = (CS + K)^{-1}F(S)$$

From which

$$(CS + K) = \begin{bmatrix} 8S+2 & 4S-2 & 0 \\ 4S-2 & 16S+4 & 4S-2 \\ 0 & 4S-2 & 8S+2 \end{bmatrix}$$

$$(CS+K)^{-1} =$$

$$\frac{1}{192S(4S+1)(S+1)} \begin{bmatrix} 4(28S^2+20S+1) & -4(2S-1)(4S+1) & (4S-2)^2 \\ -4(2S-1)(4S+1) & (8S+2)^2 & -(8S+2)(4S-2) \\ 4(2S-1)^2 & -(8S+2)(4S-2) & 4(28S^2+20S+1) \end{bmatrix}$$

Also,

$$\{F(s)\}^T = [5/S \quad 0 \quad 0]$$

Multiplying $(CS+K)^{-1}\{F(s)\}$ gives

$$T(s) = \left\{ \begin{array}{l} \frac{28s^2+20s+1}{(4s+1)(s+1)s^2} \\ \frac{1-2s}{(s+1)s^2} \\ \frac{(2s-1)^2}{(4s+1)(s+1)s^2} \end{array} \right\} \quad (4.3)$$

Taking the inverse Laplace transform from (4.3), gives the nodal temperature distributions.

$$T_1(t) = 5/48(15 + t - 12e^{-.25t} - 3e^{-t})$$

$$T_2(t) = 5/48(-3 + t + 3e^{-t}) \quad (4.4)$$

$$T_3(t) = 5/48(-9 + t + 12e^{-.25t} - 3e^{-t})$$

The nodal temperature distributions obtained using (4.4) are shown in Figure 4.2. The temperature history for node two and three have negative values. Since the equations in (4.4) are the analytical solutions to the system of ODE's it must be concluded that the consistent formulation produces unrealistic results at least for the first few time intervals.

4.1.2 Lumped Formulation

The use of lumped heat capacitance matrix saves considerable computational efforts in determining the nodal temperature $\{T\}$. In this case, $[C]$ is

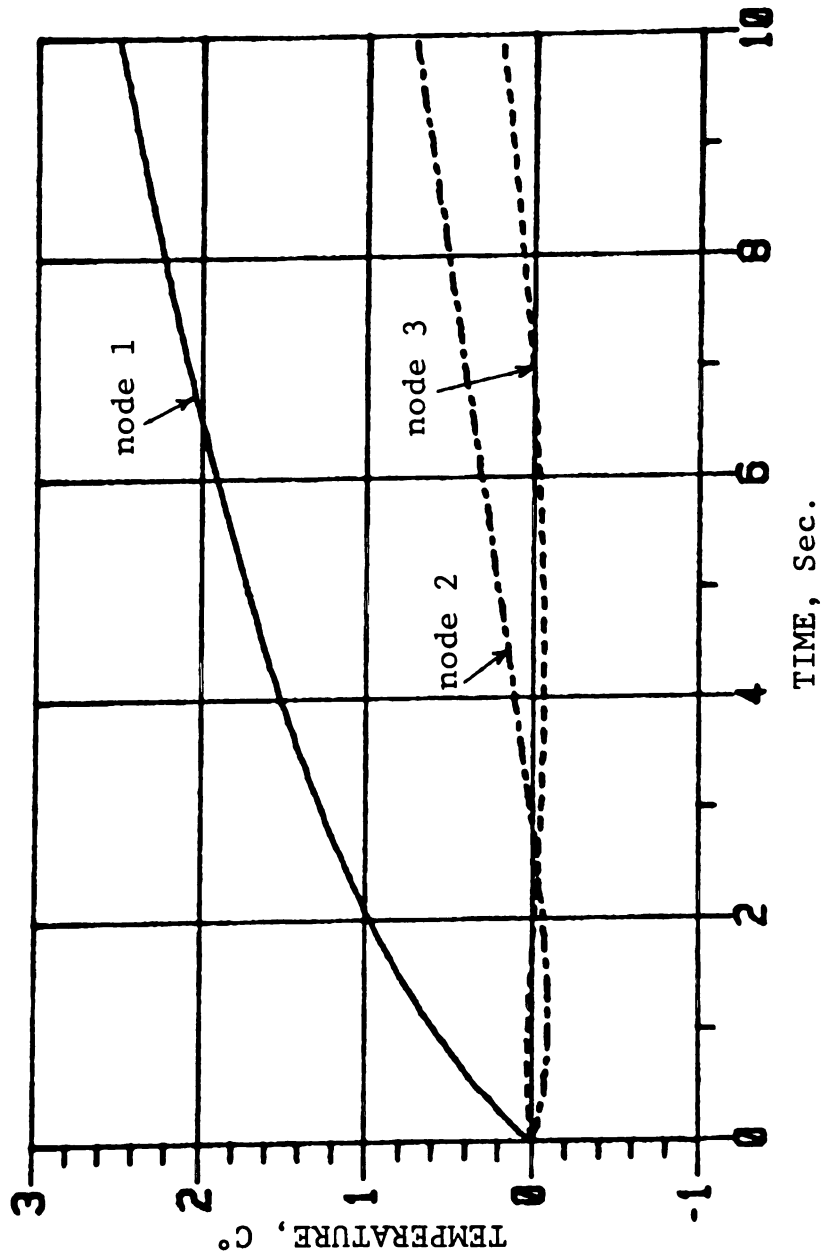


Figure 4.2 Nodal temperatures for the consistent formulations.
(Analytical Solutions)

$$[C] = \begin{bmatrix} 12 & 0 & 0 \\ 0 & 24 & 0 \\ 0 & 0 & 12 \end{bmatrix}$$

and the Laplace transform method gives

$$\begin{aligned} T_1(t) &= 5/48(15 + t - 12\bar{e}^{t/6} - 3\bar{e}^{t/3}), \\ T_2(t) &= 5/48(-3 + t + 3\bar{e}^{t/3}), \\ T_3(t) &= 5/48(-9 + t + 12\bar{e}^{t/6} - 3\bar{e}^{t/3}), \end{aligned} \quad (4.5)$$

The nodal temperatures for various times are plotted in Figure 4.3 for comparison with the consistent formulation. All of the nodal temperatures are positive. These two numerical approximations (lumped and consistent) produce the same results for large values of time. This fact can be seen from the equations in (4.4) and (4.5). The corresponding terms are identical except the exponents associated with the exponential terms. There is a significant difference between the solutions, however, for small time values.

4.2 OPERATING REGION FOR A ONE-DIMENSIONAL UNIFORM GRIDS

The criteria presented in chapter III was used to analyze a group of uniform grids to determine the operating regions relative to the time step. The one-dimensional

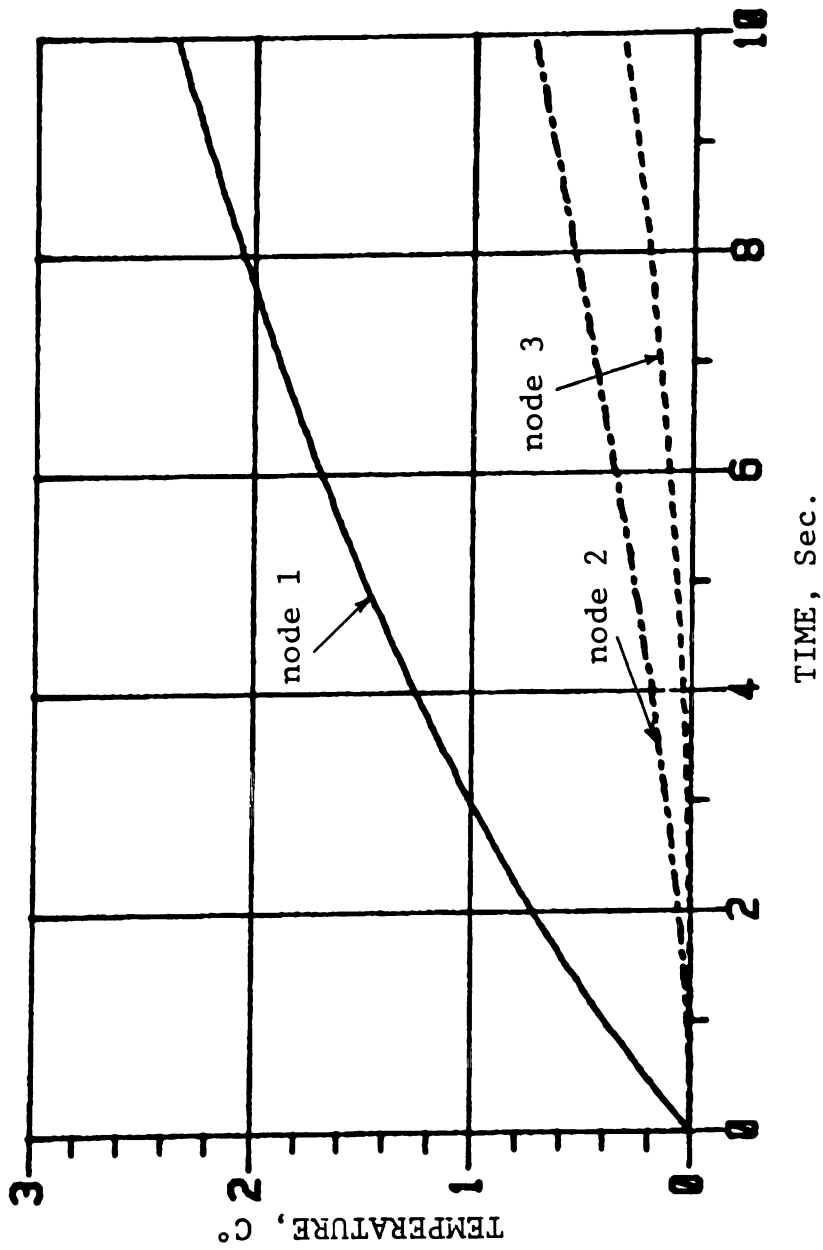


Figure 4.3 Nodal temperatures for the lumped formulations.
(Analytical Solutions)

linear grid is discussed here. A pair of two-dimensional grids are discussed in the following sections.

4.2.1 Consistent Formulations

The Fourier's heat conduction equation for a one-dimensional isotropic region is

$$\frac{\partial^2 T(X,t)}{\partial X^2} = \frac{1}{\alpha} \frac{\partial T(X,t)}{\partial t}, \quad 0 \leq X \leq L \quad (4.6)$$

where α is thermal diffusivity. Subdividing the region into identical linear elements gives the element matrices, Segerlind (1976).

$$[k^{(e)}] = \frac{\alpha}{\Delta x} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}; \text{ and } [C^{(e)}] = \frac{\Delta x}{6} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$$

From which Δx is the element length. The global matrices $[K]$ and $[C]$ for a finite number of identical elements (three elements) are

$$[K] = \frac{\alpha}{\Delta x} \begin{bmatrix} 1 & -1 & & \\ -1 & 2 & -1 & \\ & -1 & 2 & -1 \\ & & -1 & 1 \end{bmatrix}; \quad [C] = \frac{\Delta x}{6} \begin{bmatrix} 2 & 1 & & \\ 1 & 4 & 1 & \\ & 1 & 4 & 1 \\ & & 1 & 2 \end{bmatrix}$$

Substituting the above matrices into (2.33) gives

$$\begin{aligned}
& \begin{bmatrix} \frac{2}{6} + r\theta & \frac{1}{6} - r\theta & & \\ \frac{1}{6} - r\theta & \frac{4}{6} + 2r\theta & \frac{1}{6} - r\theta & \\ & \frac{1}{6} - r\theta & \frac{4}{6} + 2r\theta & \frac{1}{6} - r\theta \\ & & \frac{1}{6} - r\theta & \frac{2}{6} + r\theta \end{bmatrix} \{T\}_{n+1} \\
& = \begin{bmatrix} \frac{2}{6} - r(1-\theta) & \frac{1}{6} + r(1-\theta) & & \\ \frac{1}{6} + r(1-\theta) & \frac{4}{6} - 2r(1-\theta) & \frac{1}{6} + r(1-\theta) & \\ & \frac{1}{6} + r(1-\theta) & \frac{4}{6} - 2r(1-\theta) & \frac{1}{6} + r(1-\theta) \\ & & \frac{1}{6} + r(1-\theta) & \frac{2}{6} - r(1-\theta) \end{bmatrix} \{T\}_n
\end{aligned} \tag{4.7}$$

where $r = \alpha \Delta t / (\Delta x)^2$.

The stability criteria for uniform grids can be obtained from the solution of (4.7) using separation of variables, Lemmon (1969). The matrix stability method was used because of its adaptability to any type of complicated problem.

As mentioned in Chapter II, the largest eigenvalue of

$$[K]\{X\} = \lambda [C]\{X\} \tag{4.8}$$

is needed to determine the stability and non-oscillation criteria. The maximum eigenvalue, λ_N , for a uniform grid is

$$\lambda_N = \frac{12\alpha}{(\Delta x)^2} \tag{4.9}$$

and it is independent of number of elements (This property is shown in Chapter VI). Substituting (4.9) into (2.65) and (2.66) gives the following inequalities for the stability and non-oscillation requirements.

$$\text{Stability requirement} \quad r < \frac{1}{6(1-2\theta)} \quad (4.10)$$

$$\text{Non-oscillation requirement} \quad r < \frac{1}{12(1-\theta)} \quad (4.11)$$

For $\theta = 1$, the system does not oscillate. For values of $\theta > 1/2$, the system is unconditionally stable regardless of the integration time step and physical properties. The above inequalities are plotted in Figure 4.4. It can be seen from this plot the Euler's method ($\theta = 0$) requires the smallest value for Δt in order the system be stable. Therefore, this scheme is the most restrictive one for solving transient field problems.

Dusinberre's criteria requires negative off-diagonal coefficients in $[A]$ and positive elements in $[P]$. Lemmon, (1969) states that the coefficients in (4.7) have to be positive which is not the correct interpretation of Dusinberre's criteria. Dusinberre's analysis requires

$$1/6 - r\theta \leq 0 \quad \text{or} \quad r \geq 1/6\theta \quad (4.12)$$

and

$$2/6 - r(1-\theta) \geq 0, \quad \text{or} \quad r \leq \frac{1}{3(1-\theta)} \quad (4.13)$$

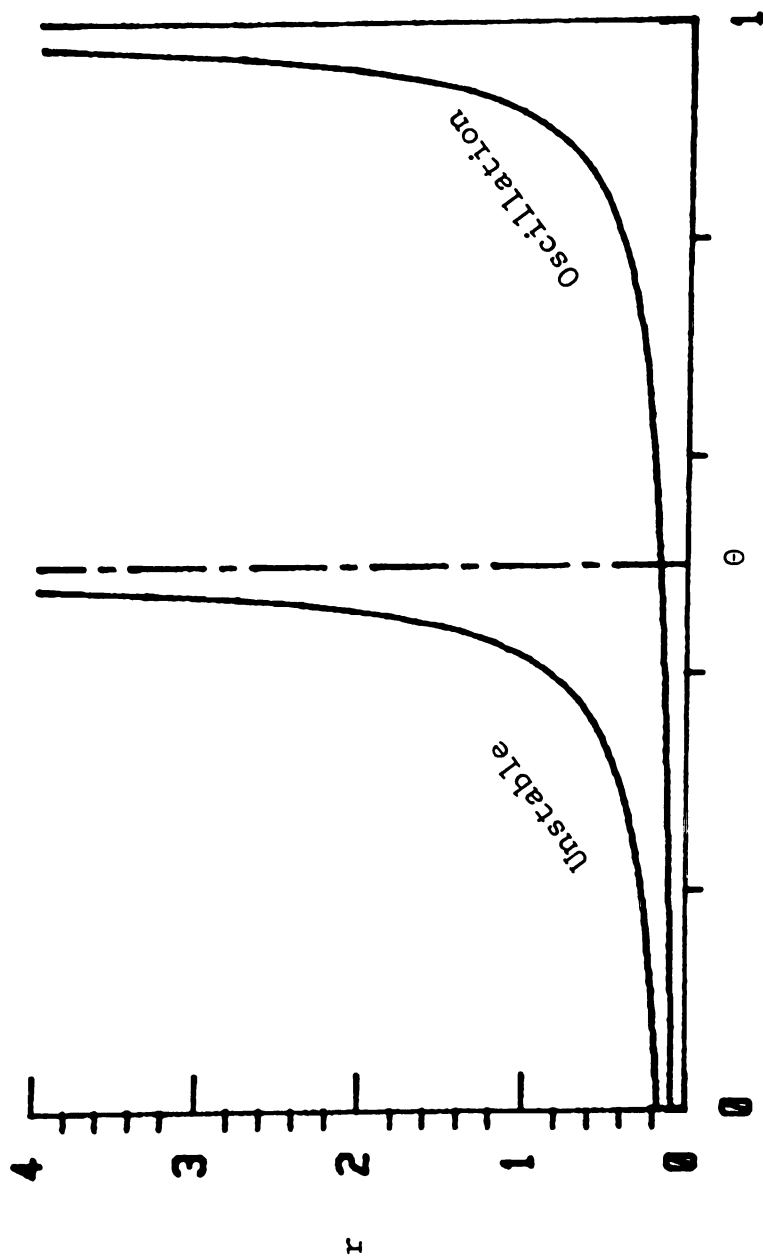


Figure 4.4 Stability and non-oscillation criteria (Consistent).

Equations (4.11) along with (4.12) and (4.13) are plotted in Figure 4.5 to obtain the operating region for a non-oscillatory system and similarly inequalities (4.10), (4.12), and (4.13) are plotted in Figure 4.6 to show the operation region for a stable system. It is clear that Euler's method will not yield good results because it is not in the operating region for the values of θ less than $1/6$.

4.2.2 Lumped Formulation

The element heat capacitance matrix, $[c^{(e)}]$, for linear temperature distribution and a lumped formulation is

$$[C^{(e)}] = \frac{\Delta x}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

and the global matrix $[C]$ for three identical element is

$$[C] = \frac{\Delta x}{2} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

The global conductivity matrix $[K]$, remains unchanged and is the same as that for consistent formulations. Following the same procedure illustrated for consistent formulations, the finite difference recurrence formula for the lumped case is

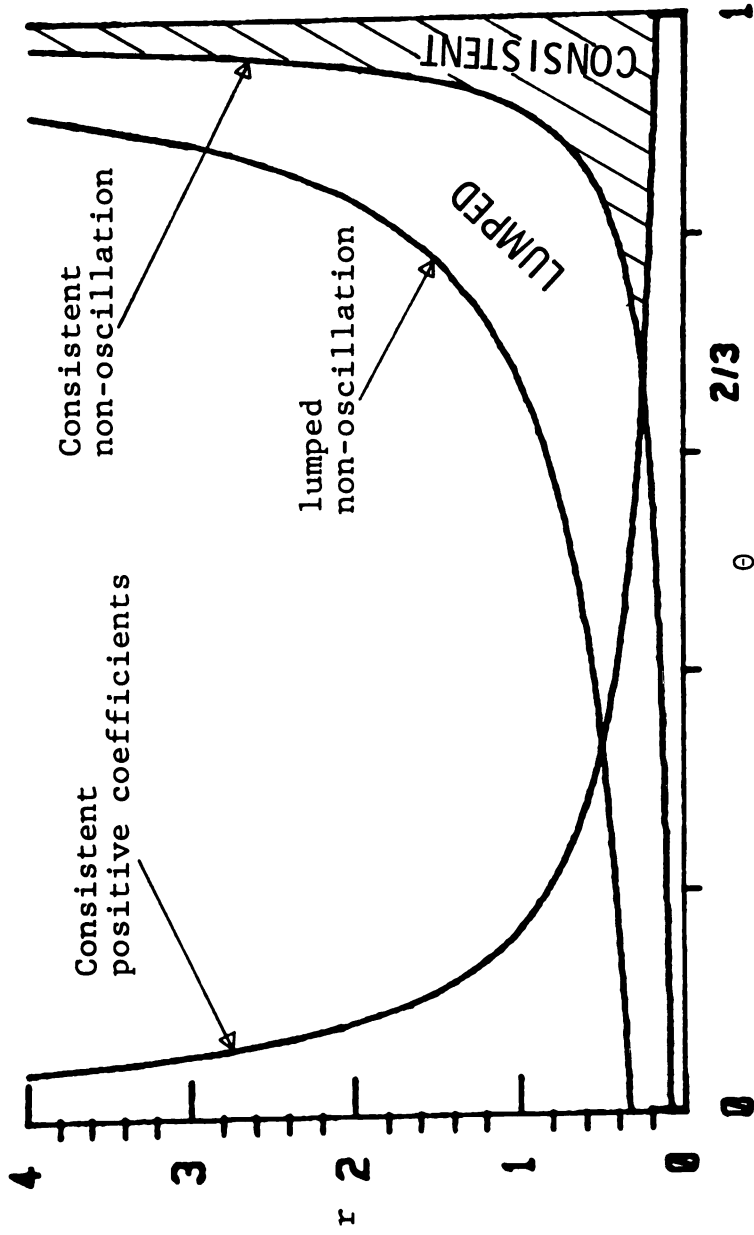


Figure 4.5 Non-oscillation region (Consistent).

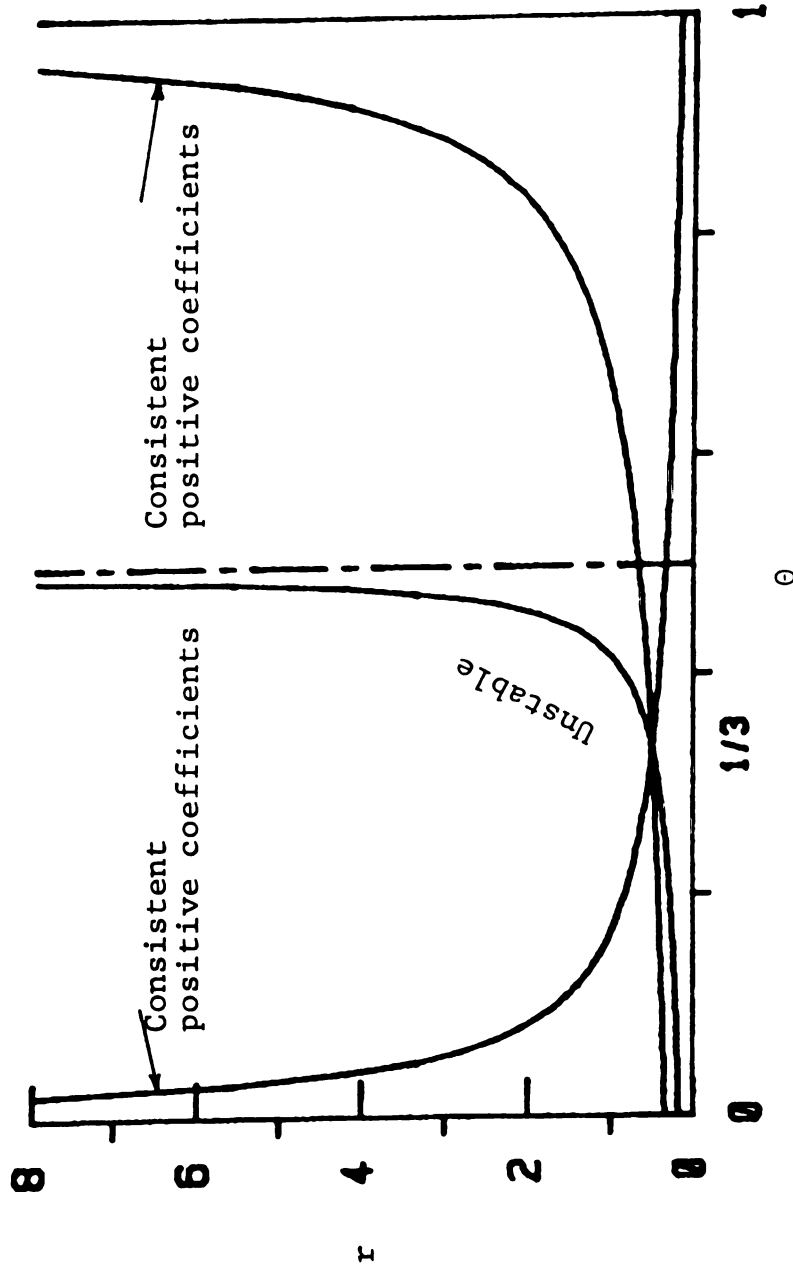


Figure 4.6 Stable operating region for consistent formulation.

$$\begin{bmatrix}
 1 + 2r\theta & -2r\theta & & \\
 -2r\theta & 2 + 4r\theta & -2r\theta & \\
 & -2r\theta & 2 + 4r\theta & -2r\theta \\
 & & -2r\theta & 1 + 2r\theta
 \end{bmatrix} \{T\}_{n+1}$$

$$\begin{bmatrix}
 1 - 2r(1-\theta) & 2r(1-\theta) & & \\
 2r(1-\theta) & 2 - 4r(1-\theta) & 2r(1-\theta) & \\
 & 2r(1-\theta) & 2 - 4r(1-\theta) & 2r(1-\theta) \\
 & & 2r(1-\theta) & 1 - 2r(1-\theta)
 \end{bmatrix} \{T\}_n$$
(4.14)

The largest eigenvalue of the system (4.8) is

$$\lambda_N = \frac{4\alpha}{(\Delta x)^2} \quad (4.15)$$

Therefore, the non-oscillation, stability and Dusiinberre's requirements are

$$\text{non-oscillation requirement} \quad r < \frac{1}{4(1-\theta)} \quad (4.16)$$

$$\text{stability requirement} \quad r < \frac{1}{2(1-2\theta)} \quad (4.17)$$

$$\text{Dusiinberre's requirement} \quad r < \frac{1}{2(1-\theta)} \quad (4.18)$$

The operating region for non-oscillatory and Dusiinberre criteria are determined by the single inequality of (4.16). This operating region is shown in Figure 4.7 along with the same conditions (Dusiinberre and non-oscillation requirements) for consistent formulations. It shows that consistent formulation is more restrictive relative to selecting a time step than the lumped formulation.

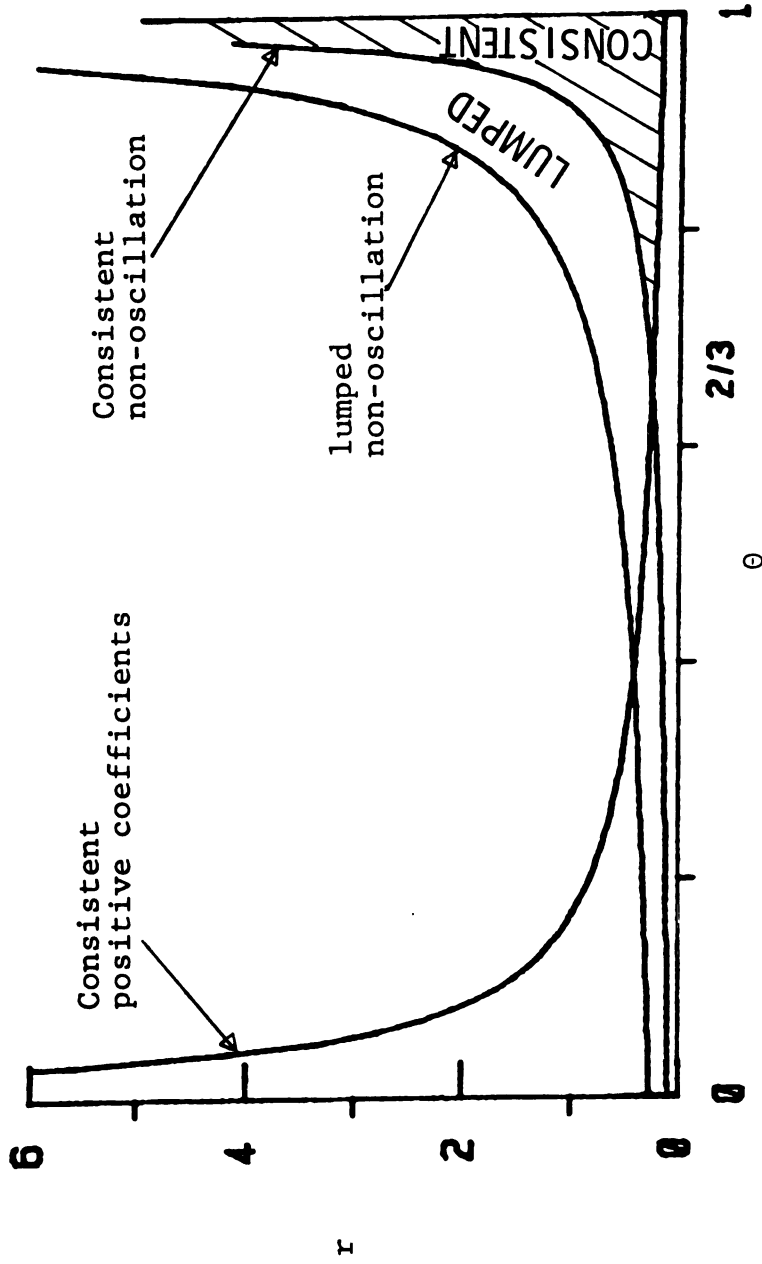


Figure 4.7 Operating regions for lumped and consistent formulations.

4.3 OPERATING REGION FOR TWO DIMENSIONAL UNIFORM GRIDS

A pair of uniform two-dimensional grids were analyzed using the criteria stated in Chapter III. One grid consisted of square elements while the other consisted of equilateral triangular elements.

4.3.1 Square Grids

A typical set of elements for a uniform square grid are shown in Figure 4.8. The element matrices for each element are

$$[K^{(e)}] = \frac{D}{6} \begin{bmatrix} 4 & -1 & -2 & -1 \\ -1 & 4 & -1 & -2 \\ -2 & -1 & 4 & -1 \\ -1 & -2 & -1 & 4 \end{bmatrix};$$

and

$$[C^{(e)}] = \frac{\rho c A}{36} \begin{bmatrix} 4 & 2 & 1 & 2 \\ 2 & 4 & 2 & 1 \\ 1 & 2 & 4 & 2 \\ 2 & 1 & 2 & 4 \end{bmatrix}$$

where A is the area of the square and D is thermal conductivity. The largest eigenvalue of the system (4.8), λ_n , is

$$\lambda_n = \frac{24D}{\rho c A} \quad (4.19)$$

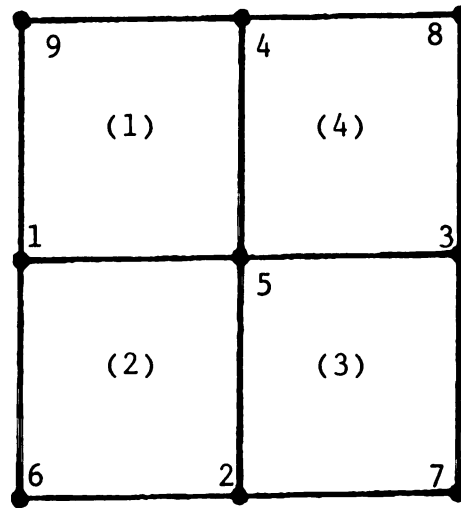


Figure 4.8 A grid of four square elements.

Substituting the computed value into (2.66) gives the non-oscillation criteria

$$r < \frac{1}{24(1-\theta)} \quad (4.20)$$

where $r = (D\Delta t)/\rho cA$.

Dusiberre's criteria is related to the coefficients in global matrices [A] and [P]. Using the direct stiffness procedure, the equation for the center node is

$$\begin{aligned} & \frac{\rho cA}{36}(4\dot{T}_1 + 4\dot{T}_2 + 4\dot{T}_3 + 4\dot{T}_4 + 16\dot{T}_5 + \dot{T}_6 + \dot{T}_7 + \dot{T}_8 + \dot{T}_9) \\ & + \frac{D}{3}(-T_1 - T_2 - T_3 - T_4 + 8T_5 - T_6 - T_7 - T_8 - T_9) = 0 \end{aligned} \quad (4.21)$$

The evaluation criteria derived in Chapter III, requires the positive diagonals and negative off-diagonal coefficients in [A] and positive coefficients in matrix [P]. These requirements are satisfied when r and θ satisfy the inequalities

$$r > \frac{1}{3\theta} ; \text{ for [A]} \quad (4.22)$$

$$r < \frac{1}{6(1-\theta)} ; \text{ for [P]} \quad (4.23)$$

The element heat capacitance matrix for the lumped formulations is

$$[C^{(e)}] = \frac{\rho c A}{4} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

which from the eigenvalue analysis yields the inequality

$$r < \frac{1}{4(1-\theta)} \quad (4.24)$$

for the non-oscillation criteria. The allowable time step for the lumped formulation is six times greater than for the consistent formulation.

A similar set of computations gives the central node equation as

$$\frac{\rho c A}{4}(4\dot{T}_5) + \frac{D}{3}(-T_1 - T_2 - T_3 - T_4 + 8T_5 - T_6 - T_7 - T_8 - T_9) = 0$$

which Dusiberre's Criteria have already been met by (4.24). The operating region for the lumped and consistent formulations are plotted in Figure 4.9. This figure shows, that the consistent formulation is highly restrictive. A value of θ exceeding .88 must be used to satisfy all of the criteria.

4.3.2 Equilateral Triangular Grids

A uniform triangular grids was studied using the six elements shown in Figure 4.10. The element stiffness matrix is

$$[k^{(e)}] = \frac{D}{2\sqrt{3}} \begin{bmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{bmatrix}$$

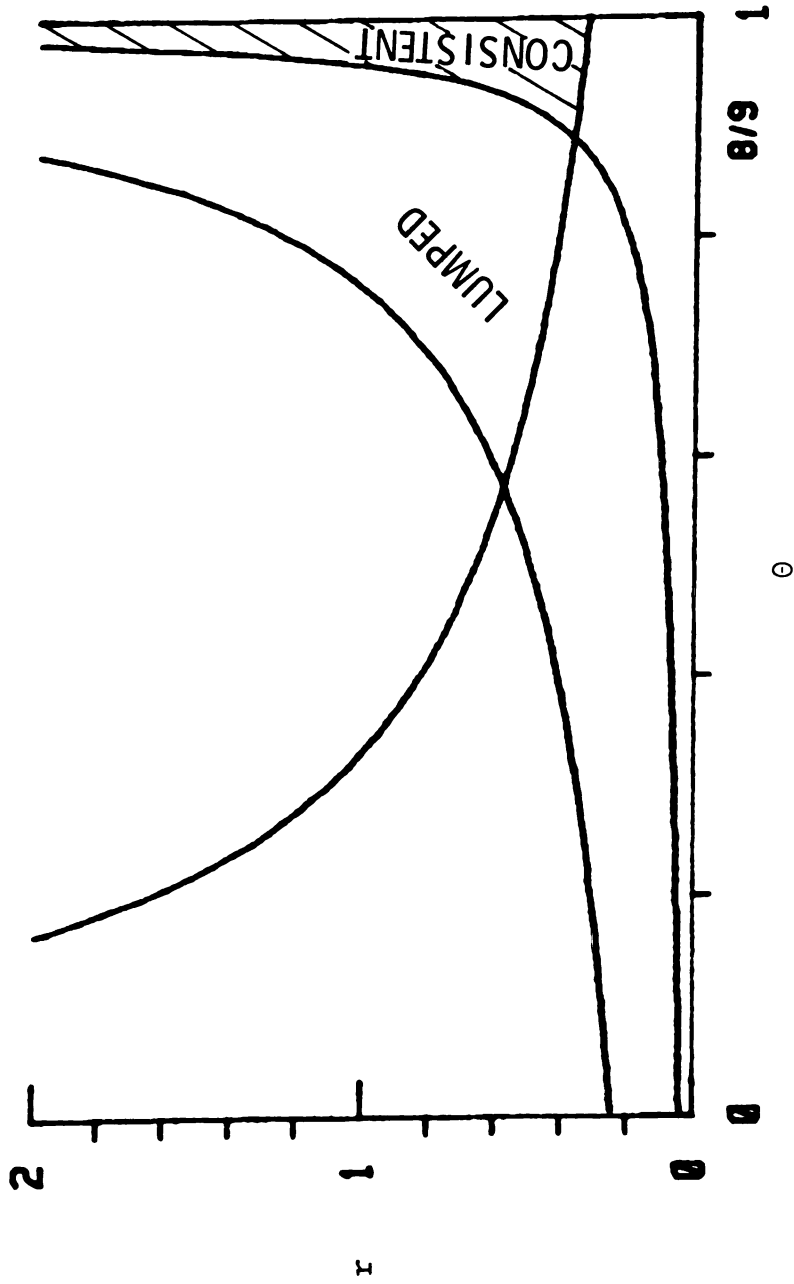


Figure 4.9 Operating regions for square grids.

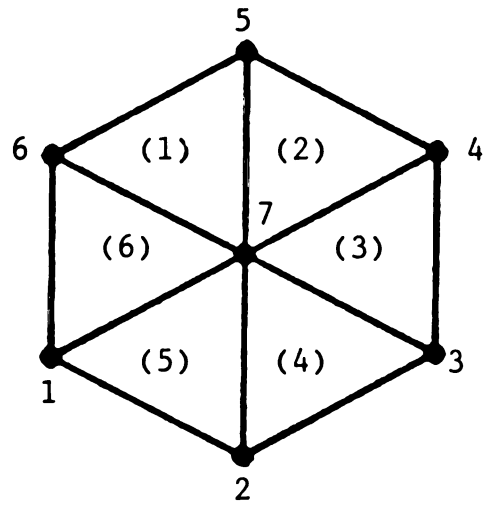


Figure 4.10 Equilateral triangular grids.

while the consistent and lumped forms of the capacitance matrices are

$$[C^{(e)}] = \frac{\rho c A}{12} \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix} ; \text{ and } [C^{(e)}] = \frac{\rho c A}{3} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

respectively.

The non-oscillation criterion requires the maximum eigenvalue, λ_N , of the system $[K]\{X\} = \lambda[C]\{X\}$. The value of

$$\lambda_N = \frac{6\sqrt{3}D}{\rho c A} \quad (4.25)$$

for the consistent formulation, and

$$\lambda_N = \frac{3\sqrt{3}}{2\rho c A} \quad (4.26)$$

for the lumped formulation. Therefore, the non-oscillation criteria for each case may be obtained by introducing (4.25) or (4.26) into (2.66) for consistent and lumped formulations. Means

$$r < \frac{\sqrt{3}}{18(1-\theta)} \quad \text{consistent non-oscillation criteria} \quad (4.27)$$

$$r < \frac{2\sqrt{3}}{9(1-\theta)} \quad \text{lumped non-oscillation criteria} \quad (4.28)$$

The assembly of the element matrices using the direct stiffness procedure produces the nodal equations (node seven)

$$\frac{\rho c A}{12} (2\dot{T}_1 + 2\dot{T}_2 + 2\dot{T}_3 + 2\dot{T}_4 + 2\dot{T}_5 + 2\dot{T}_6 + 12\dot{T}_7) \\ + \frac{D}{2\sqrt{3}} (-2T_1 - 2T_2 - 2T_3 - 2T_4 - 2T_5 - 2T_6 + 12T_7) = 0$$

for the consistent formulation and

$$\frac{\rho c A}{3} (6\dot{T}_7) + \frac{D}{2\sqrt{3}} (-2T_1 - 2T_2 - 2T_3 - 2T_4 - 2T_5 - 2T_6 + 12T_7) = 0$$

for the lumped formulation. The following extra inequality results when Dusiberre's criteria are applied to these equations,

$$r > \frac{\sqrt{3}}{6} \quad ; \text{ for consistent [A]} \quad (4.29)$$

Figure 4.11 shows the operating regions for equilateral triangle grids for consistent and lumped formulations. It shows that the consistent formulation is highly restrictive. The inequalities are satisfied only for values of θ greater than 0.75.

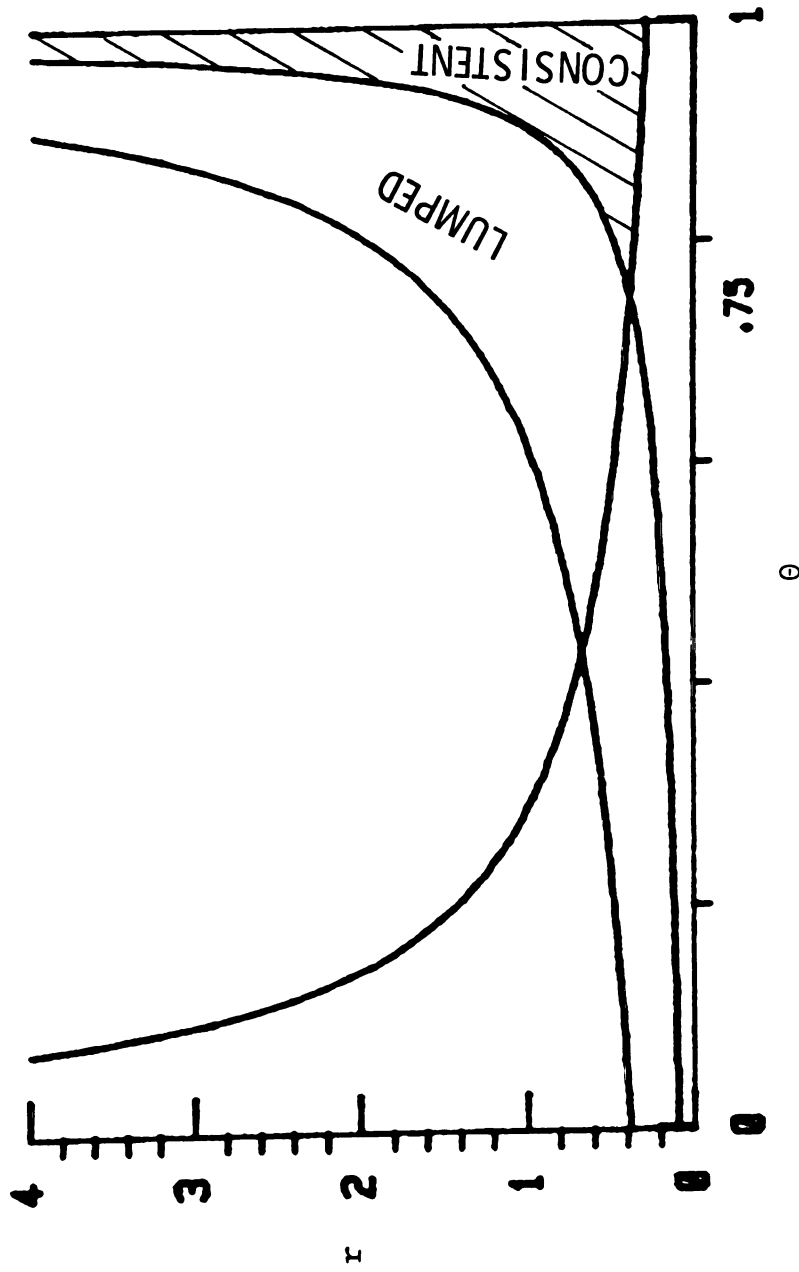


Figure 4.11 Operating regions for equilateral triangular grids.

CHAPTER V

ACCEPTABLE ELEMENTS

One aspect of this study was to investigate which elements are appropriate for a finite element discretization. Elements which fail Dusenberre's Criteria produce mixed coefficients in the general difference equation (2.41) and give results which violate physical reality. A group of the commonly used one- and two-dimensional elements were analyzed relative to Dusenberre's Criteria. The analysis was restricted to the lumped formulation.

5.1 LINEAR ONE-DIMENSIONAL ELEMENT

The element matrices for the one-dimensional linear element are

$$[k^{(e)}] = \frac{\alpha}{\Delta x} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} ; \text{ and } [C^{(e)}] = \frac{\Delta x}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad (5.1)$$

The investigation of positive coefficients in Eq. (2.41) is straight forward. The off-diagonal terms in $[k^{(e)}]$ are negative, consequently the coefficients in $[A]^{-1}$ in (2.41) are all positive. The positive coefficient rule is satisfied provided all elements of $[P]$ in (2.41) are positive.

Since $[C^{(e)}]$ is diagonal and all of the off-diagonal coefficients in $[p]$ are positive, $[P]$ has positive coefficients.

5.2 QUADRATIC ONE-DIMENSIONAL ELEMENT

The element matrices for the one-dimensional quadratic element are (5.2)

$$[k^{(e)}] = \frac{\alpha}{\Delta x} \begin{bmatrix} 14 & -16 & 2 \\ -16 & 32 & -16 \\ 2 & -16 & 14 \end{bmatrix} ; \text{ and } [C^{(e)}] = \frac{\Delta x}{3} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

The stiffness matrix $[k^{(e)}]$ contain positive off-diagonal terms thus $[A]$ contains positive off-diagonal values and Dusenberre's Criteria is not satisfied.

It is impossible to change the positive coefficients in $[k^{(e)}]$. The shape functions for the configuration in Figure 5.1 are

$$\begin{aligned} N_i &= \left(1 - \frac{x}{\xi}\right) \left(1 - \frac{x}{L}\right) \\ N_j &= \frac{x(x - L)}{\xi(\xi - L)} \\ N_k &= \frac{x(\xi - x)}{L(\xi - L)} \end{aligned} \quad (5.3)$$

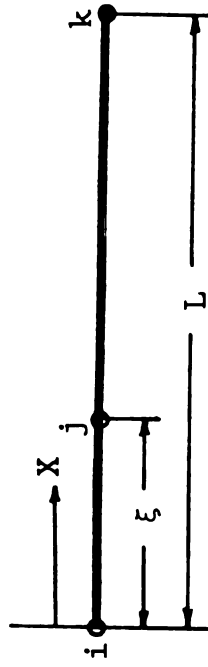


Figure 5.1 One-dimensional quadratic element.

The coefficient $k_{1,3}$ is given by

$$\begin{aligned}
 k_{1,3} &= \int_V K_x \frac{dN_i}{dx} \frac{dN_k}{dx} dv \\
 &= K_x A \int_0^L \left(\frac{2x}{\xi L} - \frac{1}{\xi} - \frac{1}{L} \right) \left(\frac{\xi}{\xi L} - \frac{2x}{L^2} \right) dx \\
 &= \frac{AK_x}{\xi L^2 (\xi - L)} (\xi L^2 - \xi^2 L - L^3/3)
 \end{aligned} \tag{5.4}$$

which is a non-negative quantity for all values of ξ between zero and 1. There is no single one-dimensional quadratic element that is useful for transient heat conduction problems.

5.3 THE LINEAR TRIANGULAR ELEMENT

The linear triangular element, Figure 5.2, has been used extensively for the solution of two-dimensional heat conduction problems. The temperature field within the element is represented by the linear polynomial.

$$T = \alpha_1 + \alpha_2 x + \alpha_3 y \tag{5.5}$$

The element matrices are (5.6)

$$[k^{(e)}] = \frac{K_x}{4A} \begin{bmatrix} b_i^2 & b_i b_j & b_i b_m \\ & b_j^2 & b_j b_m \\ \text{sym} & & b_m^2 \end{bmatrix} + \frac{K_y}{4A} \begin{bmatrix} c_i^2 & c_i c_j & c_i c_m \\ & c_j^2 & c_j c_m \\ \text{sym} & & c_m^2 \end{bmatrix}$$

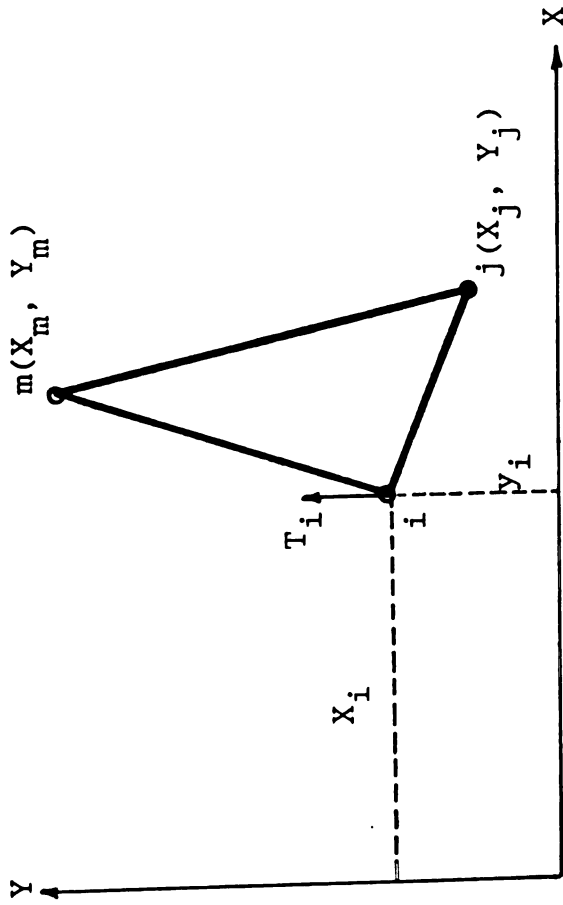


Figure 5.2 Two-dimensional triangular element.

and

$$[C^{(e)}] = \frac{\rho c A}{3} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (5.7)$$

where

$$\begin{aligned} b_i &= Y_j - Y_m ; & c_i &= X_m - X_j \\ b_j &= Y_m - Y_i ; & c_j &= X_i - X_m \\ b_m &= Y_i - Y_j ; & c_m &= X_j - X_i \end{aligned} \quad (5.8)$$

The stiffness matrix $[k^{(e)}]$, for the triangular element shown in Figure 5.3 is given by

$$\begin{aligned} [k^{(e)}] &= \frac{K_x}{2su} \begin{bmatrix} (t-u)^2 & u(t-u) & -t(t-u) \\ & u^2 & -tu \\ \text{sym} & & t^2 \end{bmatrix} \\ &+ \frac{K_y}{2su} \begin{bmatrix} s^2 & 0 & -s \\ 0 & 0 & 0 \\ -s & 0 & s^2 \end{bmatrix} \end{aligned} \quad (5.9)$$

The off-diagonal terms in (5.9) must be negative. Assuming an isotropic material, $K_x = K_y$, the negative off-diagonal criteria requires

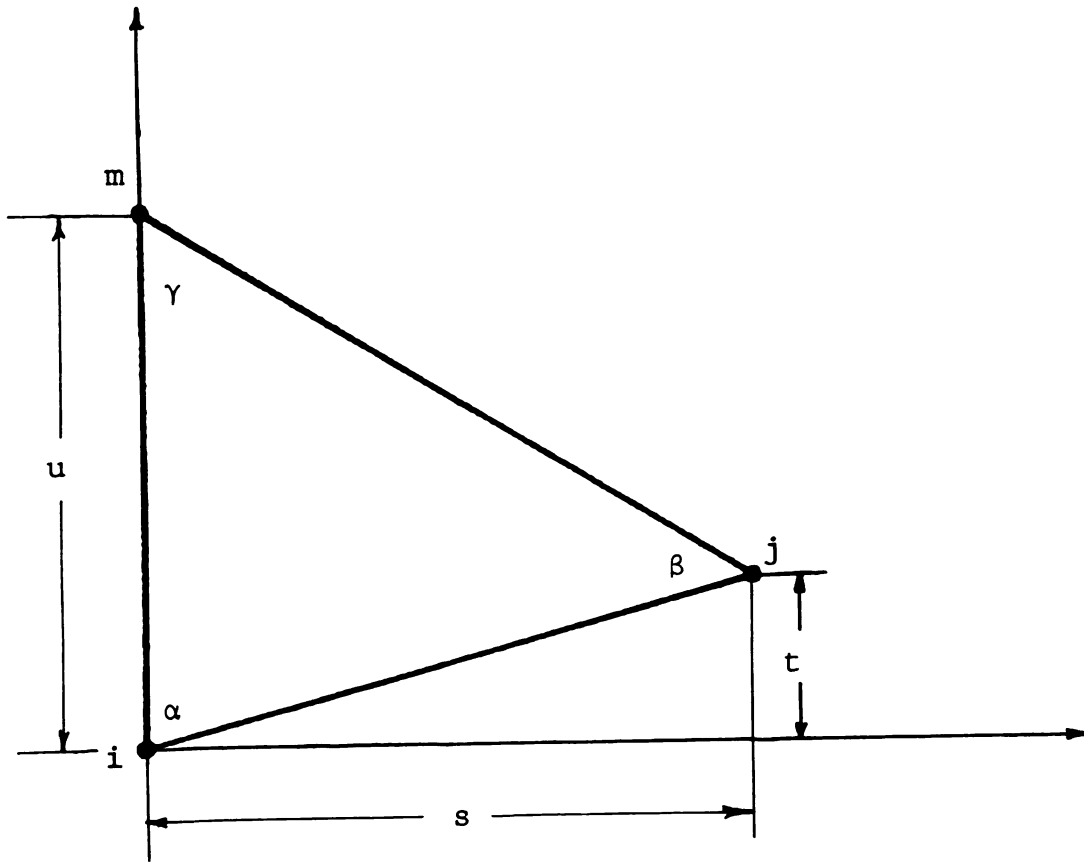


Figure 5.3 Triangular element.

$$u(t-u) < 0 \quad (5.10)$$

and

$$-tu < 0 \quad (5.11)$$

and

$$-t(t-u)-s^2 < 0 \quad (5.12)$$

where s and u are positive. The first and second inequalities require the angles γ and α to be less than 90° .

Since (5.11) requires t to be positive, the angle α must be less than or equal to 90° .

The last inequality involves the angle β . Using some trigonometric identities relating α , β and γ .

$$\tan \alpha = s/t$$

and

$$\tan \gamma = \frac{s}{u-t}$$

and

$$\tan \beta = -\tan(\alpha + \gamma) = -\frac{\tan \alpha + \tan \gamma}{1 - \tan \alpha \tan \gamma} = \frac{su}{s^2 + t^2 - tu} \quad (5.13)$$

Since $tu < s^2 + t^2$, $\tan \beta$ is positive, thus $\beta \leq 90^\circ$.

In summary, $[k^{(e)}]$ has negative off-diagonal coefficients only when all of the angles are less than or equal to 90° .

At this point, it is worthwhile to consider the relations between the allowable time step and the shape of the triangle. This study was done using the triangle shown

in Figure 5.4. The triangle has a constant area with node k moveable along a horizontal line. Therefore, the angle ϕ is related to the parameter a .

The element stiffness matrix is

$$[k^{(e)}] = \begin{bmatrix} 1 + (a+1)^2 & -a(a-1) & -1 & a-1 \\ & a^2 + 1 & & -a \\ \text{sym} & & & 1 \end{bmatrix}$$

where the conductivity in x and y directions were assumed to be the same and equal to K . The estimation of the integration time step requires the determination of the largest eigenvalue of

$$[K]\{X\} = \lambda[C]\{X\}.$$

The generalized eigenvalue problem reduces to

$$\det \begin{bmatrix} a^2 - 2a + 2 - m\lambda & -a^2 + a - 1 & a-1 \\ -a^2 + a - 1 & a^2 + 1 - m\lambda & -a \\ a-1 & -a & 1-m\lambda \end{bmatrix} = 0$$

where $m = \rho c / 3K$, and the maximum eigenvalue is

$$\lambda_n = \frac{3K}{\rho c} (a^2 - a + 2 + \sqrt{(a^2 - a + 2)^2 + 3}) \quad (5.14)$$

Eq. (5.14) is plotted in Figure 5.5. The maximum value for λ_n occurs at $a = 1/2$. The minimum value of λ_n produces the largest allowable time step. As a result, the equilateral triangle has the maximum possible ITS. The value

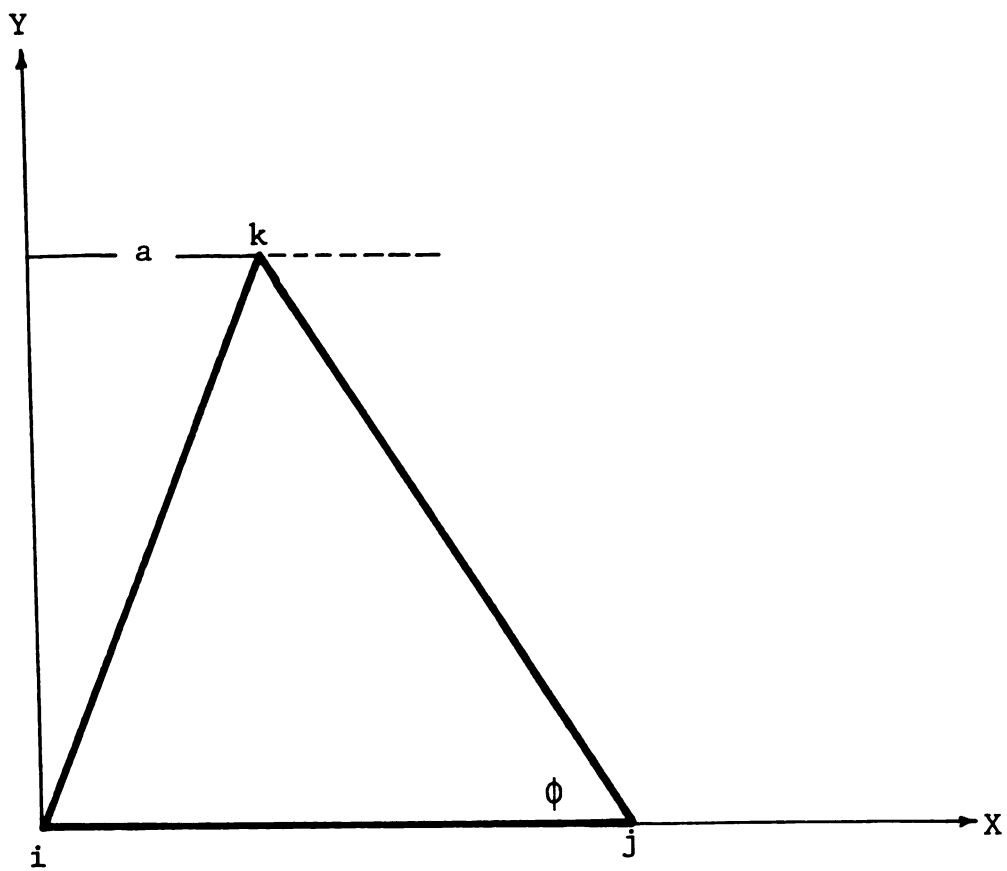


Figure 5.4 Triangular element.

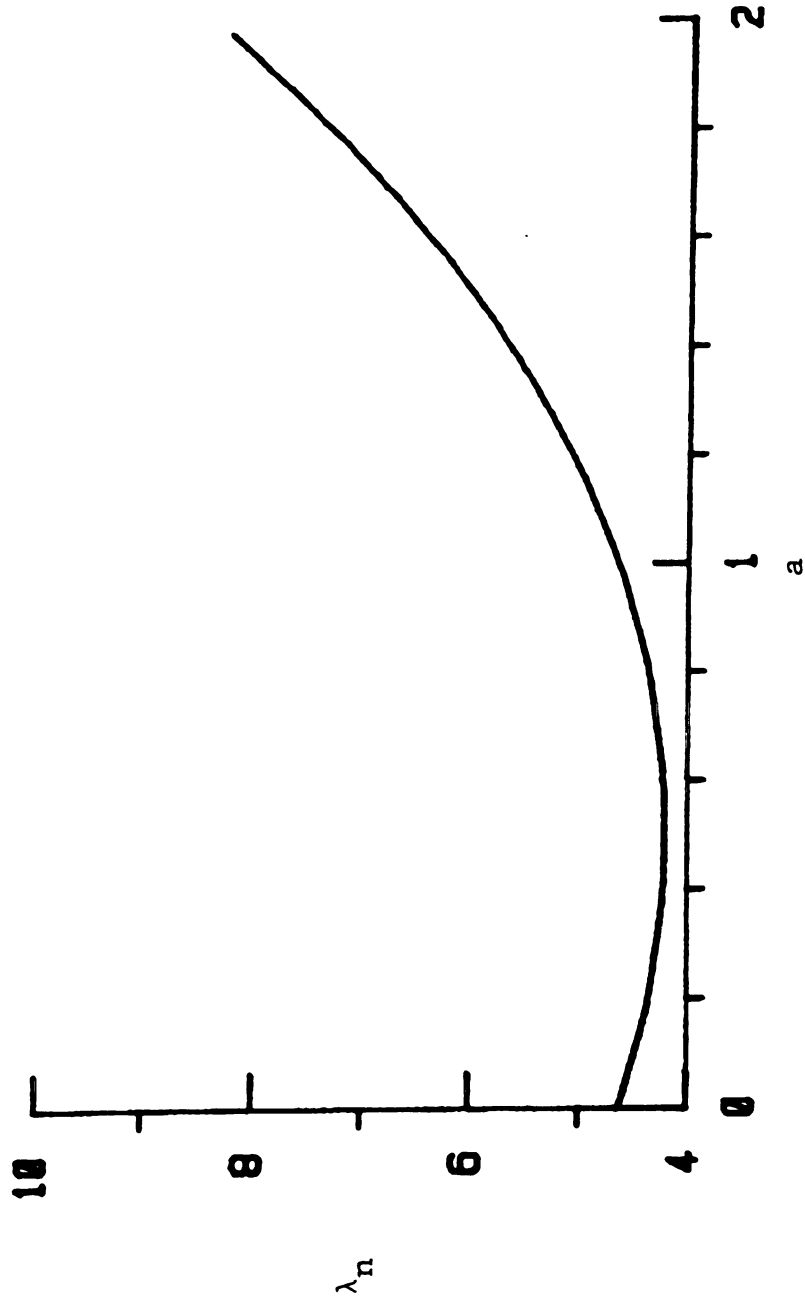


Figure 5.5 Variation of λ_n with respect to a .

of λ_n for the equilateral triangle is not appreciably different from the values for $a = 0$ or $a = 1$ which corresponds to right triangles.

5.4 TWO-DIMENSIONAL PARALLELOGRAM ELEMENT

The study of negative off-diagonal terms in the stiffness matrix of a parallelogram element, Figure 5.6, is interesting and is a starting point for a discussion of the quadrilateral and rectangular elements.

The temperature field within the element is

$$T(x,y) = \alpha_1 + \alpha_2 x + \alpha_3 y + \alpha_4 xy \quad (5.15)$$

The four constants α_i , ($i = 1, 2, 3$ and 4), are determined by nodal values T_1, \dots, T_4 .

$$\begin{aligned} T_1 &= \alpha_1 + \alpha_2 x_1 + \alpha_3 y_1 + \alpha_4 x_1 y_1 \\ T_2 &= \alpha_1 + \alpha_2 x_2 + \alpha_3 y_2 + \alpha_4 x_2 y_2 \\ T_3 &= \alpha_1 + \alpha_2 x_3 + \alpha_3 y_3 + \alpha_4 x_3 y_3 \\ T_4 &= \alpha_1 + \alpha_2 x_4 + \alpha_3 y_4 + \alpha_4 x_4 y_4 \end{aligned} \quad (5.16)$$

which yields

$$\begin{aligned} \alpha_1 &= T_1 \\ \alpha_2 &= \frac{T_2 - T_1}{a} \end{aligned} \quad (5.17)$$

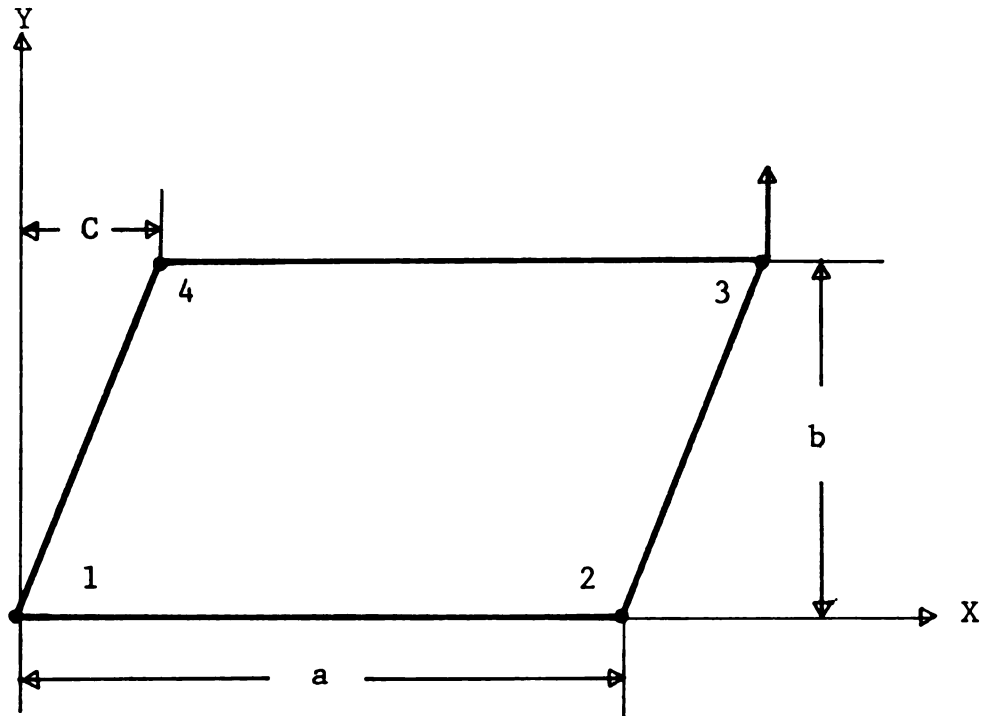


Figure 5.6 Parallelogram element.

$$\alpha_3 = \frac{a(T_4 - t_1) + c(T_4 - T_3)}{ab} \quad (5.17)$$

$$\alpha_4 = \frac{T_1 - T_2 + T_3 - T_4}{ab}$$

substituting the above values for α_1 through α_4 into (5.15) and rearrangement produces the shape functions.

$$T = \sum_{i=1}^4 T_i N_i \quad (5.18)$$

from which

$$N_1 = 1 - x/a - y/b + xy/ab$$

$$N_2 = x/a - xy/ab$$

$$N_3 = -cy/ab + xy/ab$$

$$N_4 = cy/ab - xy/ab + y/b$$

The gradient matrix $\{g\}$ is

$$\{g\} = \begin{Bmatrix} \frac{\partial T}{\partial x} \\ \frac{\partial T}{\partial y} \end{Bmatrix} = \sum_{i=1}^4 \begin{bmatrix} \frac{\partial N_i}{\partial x} \\ \frac{\partial N_i}{\partial y} \end{bmatrix} \{T^{(e)}\} \quad (5.20)$$

$$\{g\} = [B] \{T^{(e)}\}$$

where

(5.21)

$$[B] = \begin{bmatrix} (-\frac{1}{a} + \frac{y}{ab}) & (\frac{1}{a} - \frac{y}{ab}) & (\frac{y}{ab}) & -(\frac{y}{ab}) \\ (-\frac{1}{b} + \frac{x}{ab}) & (-\frac{x}{ab}) & (\frac{x}{ab} - \frac{c}{ab}) & (\frac{c}{ab} - \frac{x}{ab} + \frac{1}{6}) \end{bmatrix}$$

An individual coefficient of $[k^{(e)}]$ is obtained by evaluating

$$k_{i,j} = \int_A K_x \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} dA + \int_A K_y \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} dA$$

For example,

$$k_{1,1} = \int_A K_x \left(\frac{\partial N_1}{\partial x} \right)^2 dA + \int_A K_y \left(\frac{\partial N_1}{\partial y} \right)^2 dA$$

$$= K_x \int_0^b dy \int_{\frac{c}{b}y}^{\frac{c}{y}y+a} \left(-\frac{1}{a} + \frac{y}{ab} \right)^2 dx$$

$$+ K_y \int_0^b dy \int_{\frac{c}{6}y}^{\frac{c}{6}y+a} \left(-\frac{1}{6} + \frac{x}{ab} \right)^2 dx$$

and

$$k_{1,1} = K_x \left(\frac{b}{3a} \right) + K_y \left(\frac{c^2}{3ab} - \frac{c}{2b} + \frac{a}{3b} \right)$$

Similar computations yields element stiffness matrix as

$$\begin{aligned}
 [k^{(e)}] = & \frac{K_x}{6} \frac{b}{a} \begin{bmatrix} 2 & -2 & -1 & 1 \\ -2 & 2 & 1 & -1 \\ -1 & 1 & 1 & -1 \\ 1 & -1 & -2 & 2 \end{bmatrix} + \frac{K_y}{6} \frac{a}{b} \begin{bmatrix} 2 & 1 & -1 & -2 \\ 1 & 2 & -2 & -1 \\ -1 & -2 & 2 & 1 \\ -2 & -1 & 1 & 2 \end{bmatrix} \\
 & + \frac{K_y}{6} \frac{c^2}{ab} \begin{bmatrix} 2 & -2 & -1 & 1 \\ -2 & 2 & 1 & -1 \\ -1 & 1 & 2 & -2 \\ 1 & -1 & -2 & 2 \end{bmatrix} + \frac{K_y}{2} \frac{c}{b} \begin{bmatrix} -1 & 0 & 1 & 0 \\ 0 & 1 & 0 & -1 \\ 1 & 0 & -1 & 0 \\ 0 & -1 & 0 & 1 \end{bmatrix}
 \end{aligned} \tag{5.22}$$

Eq. (5.22) shows that the elements of the stiffness matrix are functions of the material properties and the element geometric parameters.

The diagonal terms of (5.22) are always positive and $k_{2,4}$ is always negative. The following inequalities are required for satisfaction of Dusenberre's Criteria.

$$k_{3,4} = k_{1,2} < 0 \tag{5.23a}$$

$$k_{1,3} < 0 \tag{5.23b}$$

$$k_{2,3} = k_{1,4} < 0 \tag{5.23c}$$

Taking $\frac{b}{a} = \beta$, (5.23a) becomes

$$-2\beta + \frac{1}{\beta} - \frac{2c^2}{a^2\beta} < 0$$

or

$$\frac{c^2}{a^2} + (\beta^2 - \frac{1}{2}) > 0$$

assuming $K_x = K_y$. The inequality holds for values of β greater than $\sqrt{2}/2$ and $\beta < \sqrt{2}/2$ the inequality reduces to

$$\frac{c}{a} > \sqrt{1/2 - \beta^2} \quad (5.24a)$$

Using a similar procedure (5.23b, c) simplify to

$$\frac{c}{a} < 1/2(3 - \sqrt{5 - 4\beta^2}) \quad , \text{ if } \beta < \sqrt{5}/2 \quad (5.24b)$$

and

$$\frac{c}{a} < \sqrt{2 - \beta^2} \quad ; \quad \beta < \sqrt{2} \quad (5.24c)$$

Eq. (5.23c) is not satisfied for $\beta > \sqrt{2}$ and any value of a and c .

The above inequalities are plotted in Figure 5.7.

The operating region is shaded. The ratio c/a for a rectangle is zero and the aspect ratio may vary from $\sqrt{2}/2$ to $\sqrt{2}$.

The determination of λ_n for a rectangular element indicates the square element has the smallest value and, therefore, the largest allowable time step. The analysis for the rectangular elements went as follows. The element stiffness matrix and the lumped heat capacity matrix for a rectangle with sides a and b are

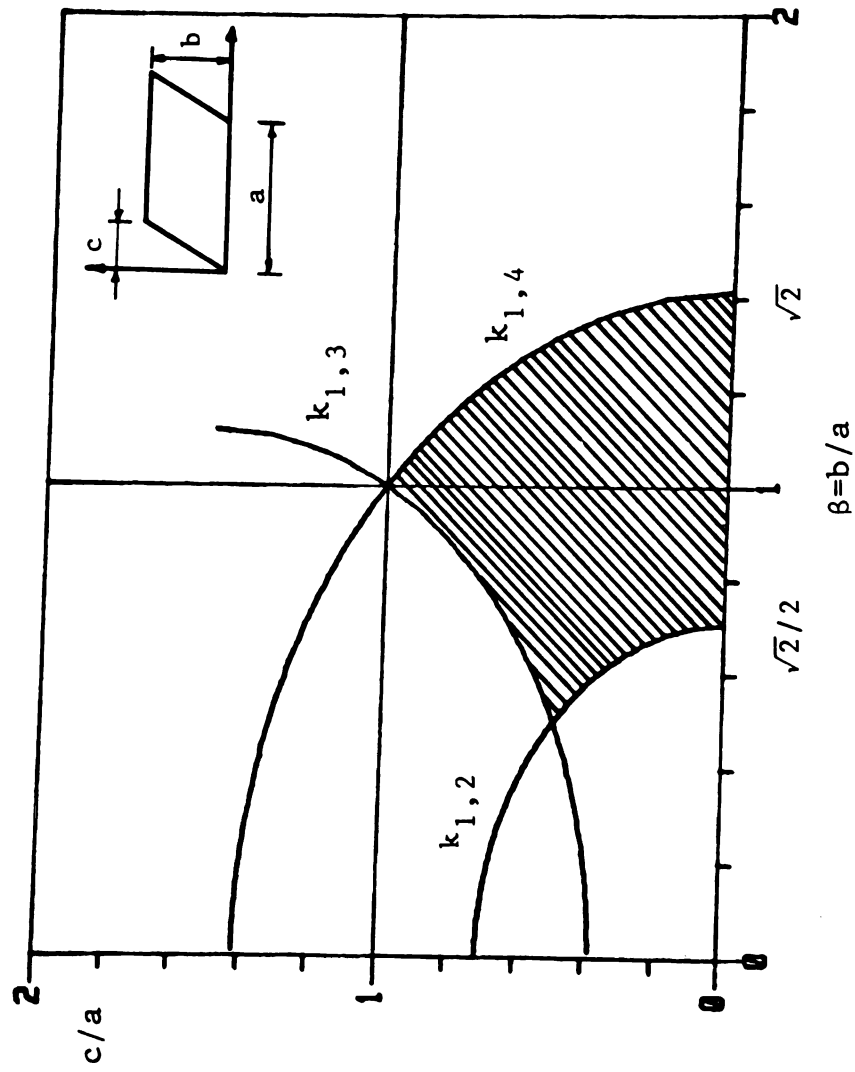


Figure 5.7 Operating region for parallelogram element.

$$[k^{(e)}] = \frac{K}{6} \begin{bmatrix} 2(\beta + \frac{1}{\beta}) & (-2\beta + \frac{1}{\beta}) & -(\beta + \frac{1}{\beta}) & (\beta - \frac{2}{\beta}) \\ (-2\beta + \frac{1}{\beta}) & 2(\beta + \frac{1}{\beta}) & (\beta - \frac{2}{\beta}) & -(\beta + \frac{1}{\beta}) \\ -(\beta + \frac{1}{\beta}) & (\beta - \frac{2}{\beta}) & 2(\beta + \frac{1}{\beta}) & (-2\beta + \frac{1}{\beta}) \\ (\beta - \frac{2}{\beta}) & -(\beta + \frac{1}{\beta}) & (-2\beta + \frac{1}{\beta}) & 2(\beta + \frac{1}{\beta}) \end{bmatrix}$$

and

$$[c^{(e)}] = \frac{\rho c A}{4} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

where K is thermal conductivity and β is the aspect ratio. The maximum eigenvalue of $[K]\{X\} = \lambda[C]\{X\}$ for above matrices can be obtained for different values of β using the computer to evaluate λ_n given β . The results have been plotted on Figure 5.8. It shows the square element has the minimum value for λ_n and therefore, the maximum allowable time step.

5.5 LINEAR QUADRILATERAL ELEMENT

A general linear quadrilateral element with a natural coordinate system is shown in Figure 5.9. The use of a natural coordinate system allows the side of the quadrilateral to rotate relative to xy coordinate system and still satisfy the continuity requirements. The shape function for this element are given by (Segerlind, 1976).

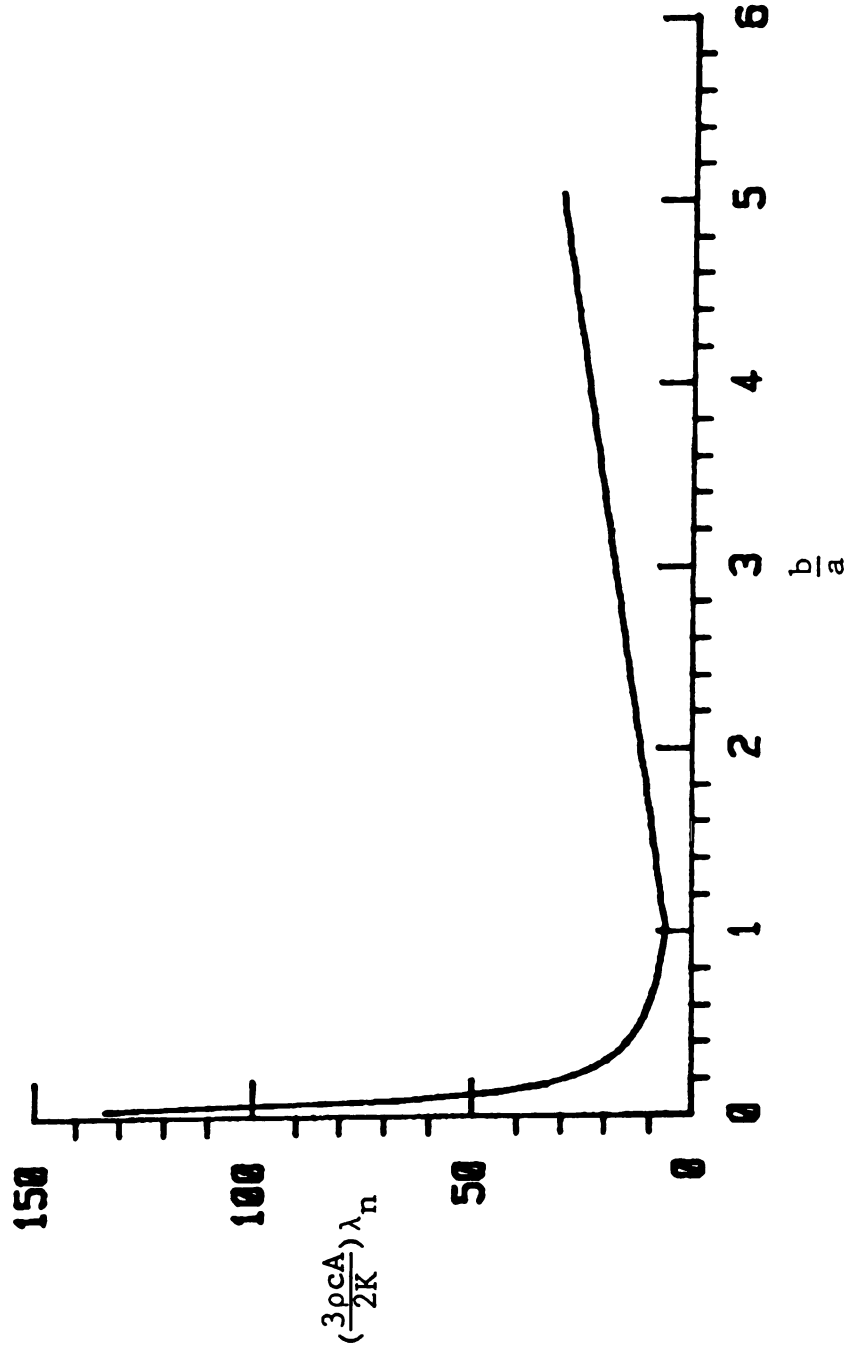


Figure 5.8 Variation of λ_n with respect to b/a .

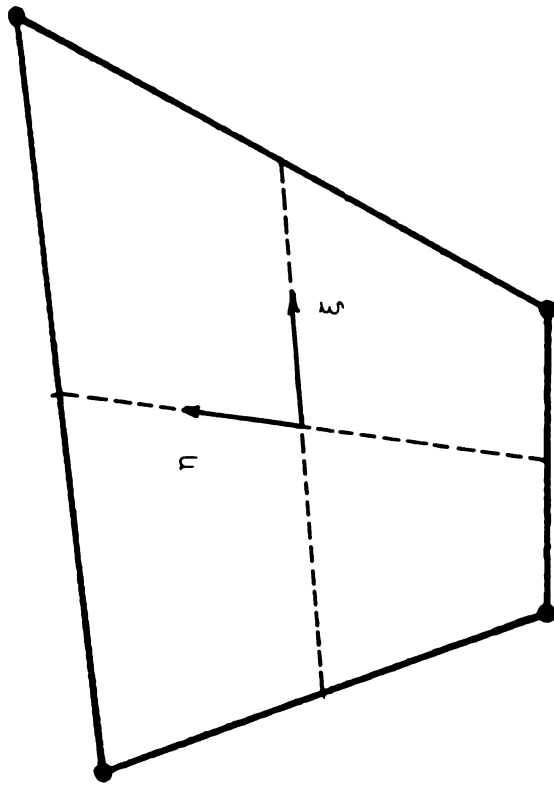


Figure 5.9 Linear quadrilateral element.

$$\begin{aligned}
 N_1 &= \frac{1}{4}(1-\xi)(1-\eta) & N_2 &= \frac{1}{4}(1+\xi)(1-\eta) \\
 N_3 &= \frac{1}{4}(1+\xi)(1+\eta) & N_4 &= \frac{1}{4}(1-\xi)(1+\eta)
 \end{aligned}
 \tag{5.25}$$

The stiffness matrix must be evaluated using numerical integration techniques. As a result, the investigation of negative off-diagonal in $[k^{(e)}]$ is not simple and straightforward. To obtain some information about the coefficients in $[k^{(e)}]$, this matrix was evaluated for some simple variations from a square. The base was fixed and the upper corners were moved together or separately to see how much the element could be deformed before positive coefficients appeared in $[k^{(e)}]$.

Figure 5.10 shows five different shapes where the quadrilateral deformed to a point where positive coefficients appear in the off-diagonal location of $[k^{(e)}]$. The coordinates of each node are shown close to the corners. Figure 5.10a shows, that the upper corner can be moved until the side is about 47 percent of its original length. Plot 5.10b shows the movement of point three in a horizontal direction to the right. The side can be increased in length and about 56 percent. Figure 5.10c indicates that node three can be moved to the left 50 percent of its original length. Figure 5.10d shows that node three can be moved along a 45 degree line (the line $y=x$) toward the origin until the square became a triangle. The last figure, 5.10e indicates a significant deformation can occur

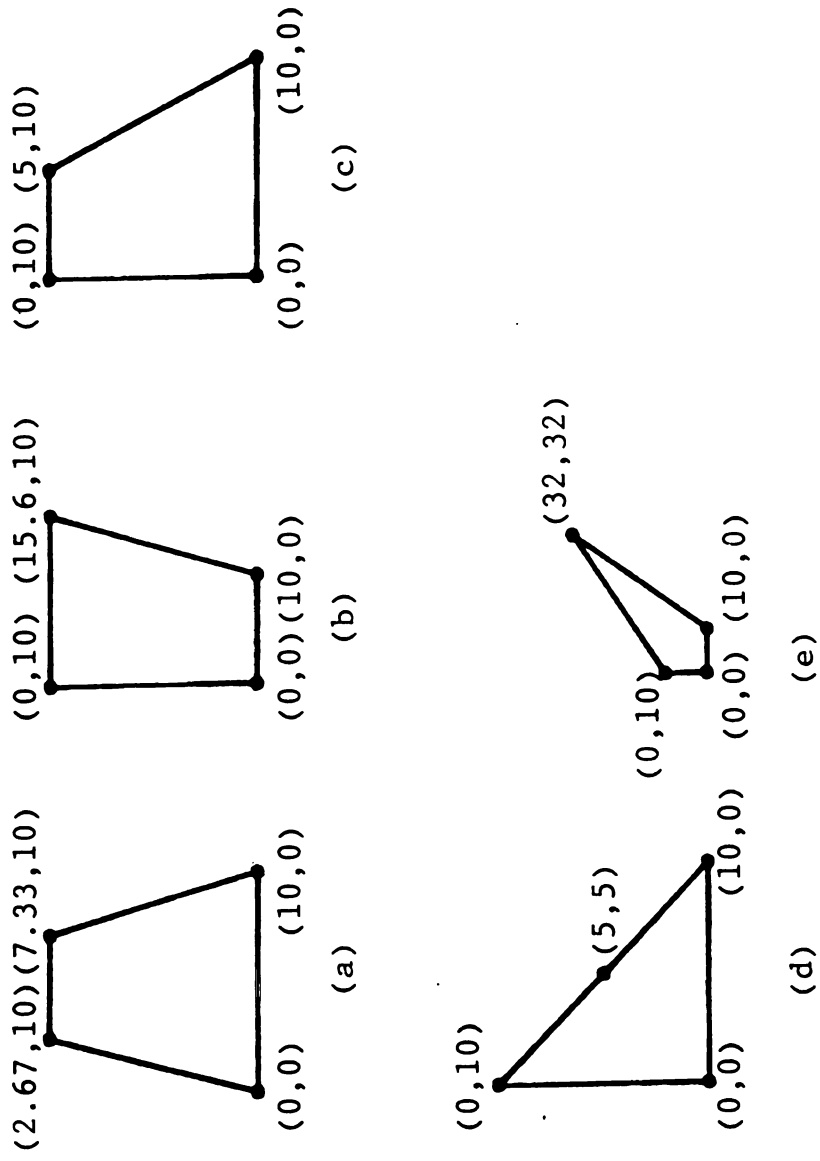


Figure 5.10 Quadrilateral elements.

along the line $y=x$ and away from the origin before positive coefficients occur in the off-diagonal values of $[k^{(e)}]$.

5.6 QUADRATIC AND CUBIC QUADRILATERAL ELEMENTS

Numerical calculation shows that the quadratic and cubic elements, both squares and equilateral triangles, have positive off-diagonal coefficients in $[k^{(e)}]$ and can not satisfy Dusenberre's Criteria. The need to numerically integrate these elements prevents an analytical investigation. Sample matrices for each type of quadratic element are given in Figure 5.11. Since the square and equilateral triangle were the optimum linear two-dimensional elements, deformed quadratic elements were not investigated.

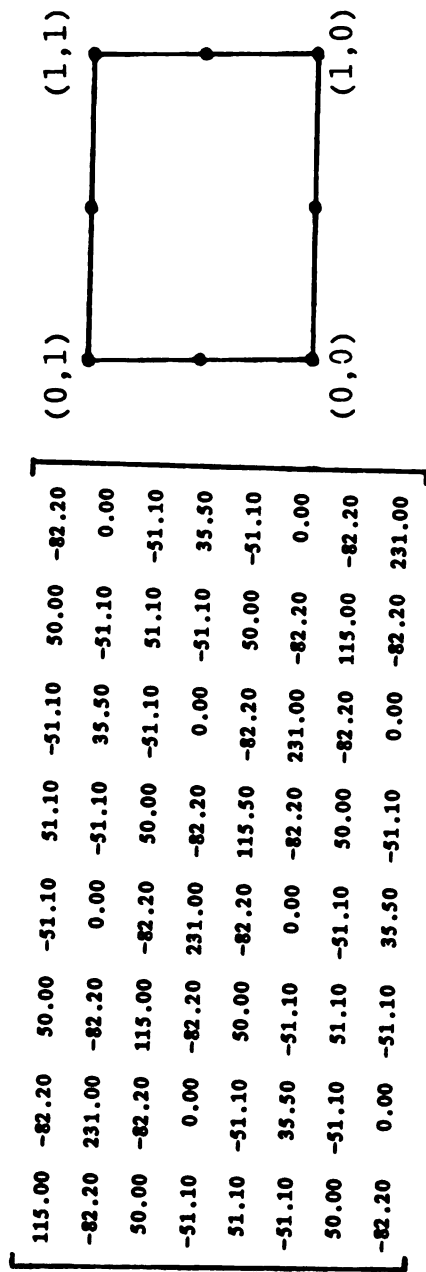
5.7 CONVECTIVE BOUNDARY CONDITIONS

The contribution of convective heat loss to the stiffness matrix is given by $\int_s h[N]^T[N] ds$. The element stiffness matrix for a one-dimensional fin problem is

$$[k^{(e)}] = \frac{AK_x}{L} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} + \frac{hpL}{6} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \quad (5.26)$$

where p is the perimeter and h is the convection coefficient.

It is clear from (5.26) that positive off-diagonal coefficients can occur in $[K^{(e)}]$ for some values of h and p . This possibility should be eliminated by using the concepts of lumping. The convection contribution should be lumped to give



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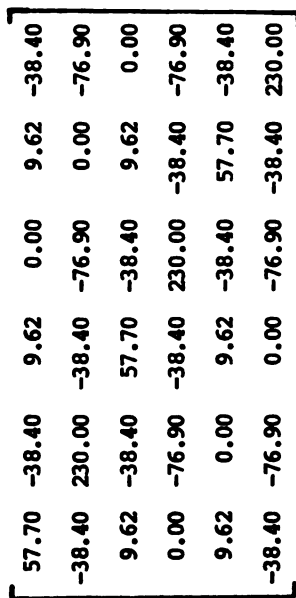
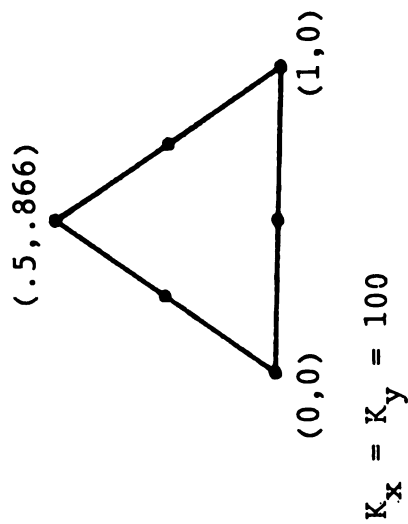


Figure 5.11 Quadratic elements with corresponding stiffness matrices.

$$[k^{(e)}] = \frac{AK_x}{L} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} + \frac{hpL}{6} \begin{bmatrix} 3 & 0 \\ 0 & 3 \end{bmatrix} \quad (5.27)$$

The off-diagonal terms remain negative and Dusiinberre's Criteria is satisfied regardless of physical properties and geometrical size.

The convection related matrices for all elements (in all dimensions) should be lumped to avoid positive off-diagonal values in $[K^{(e)}]$.

CHAPTER VI

ESTIMATION OF A TIME STEP VALUE

An estimation of an optimum time step value is necessary for efficient numerical computation. The value of the integration time step for some uniform grids is known. The difficulty arises for irregular meshes with different types of materials and boundary conditions. These grids represent the usual situation in finite element solutions.

The maximum allowable time step can be obtained by knowing the maximum eigenvalue of the system

$$[K]\{X\} = \lambda[C]\{X\} \quad (6.1)$$

This computation is not a quick one and the algebraic computations are large for a large system of equations. Consequently, the idea of an estimated value for the time step has been investigated to eliminate the eigenvalue computations. Myers(1977), based his estimation of time step on the Gerschgorin's theorem and derived the safe time step for a two dimensional region subdivided into the triangular elements. The idea of element computation of a maximum time step value has also been suggested by Welty (1974).

The methods of Myers and Welty are conservative. The idea of a subregion analysis for estimating the time step value is given in this chapter.

6.1 METHOD OF ESTIMATION

A method for estimating the maximum eigenvalue is based on the eigenvalue bound theorem for (6.1) developed by Fried (1979). In this regard, the lowest (1st) and the highest (N^{th}) eigenvalue of the global system (6.1), are denoted by λ_1 and λ_N , respectively. The bound theorem states

$$\lambda_{\min}^e \text{ (over all elements, } e) < \lambda_1$$

and (6.2)

$$\lambda_N < \lambda_{\max}^e \text{ (over all elements, } e)$$

The method of subregion analysis presented here applies the bound theorem to a group of elements which are treated as a single element. This idea is similar to the substructuring technique used in structural analysis. A group of elements are combined to make a super element.

6.2 LINEAR UNIFORM GRIDS

In a region containing similar elements, the non-oscillatory characteristics can be obtained by the analyzing of a single element. This fact is shown below for the one-dimensional case.

For
the maximum

$$\lambda_n = 12$$

which is a
matrices,

$$\{u\}^T$$

To
(6.1) wh

$$\frac{a}{\Delta x} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

this ma

$$12a/(\Delta x)$$

is the

is

$$\lambda_n$$

which

Δ

For the element matrices given in Chapter IV, page 46 the maximum eigenvalue of (6.1) on an element basis is

$$\lambda_n = 12\alpha/(\Delta x)^2 \quad (6.3)$$

which is also, one of the eigenvalue of (6.1) for the global matrices, page 46, with the following eigenvector

$$\{u\}^T = [1 \quad -1 \quad 1 \quad -1 \quad 1 \dots]$$

To show this we substitute the global matrices into (6.1) which yields

$$\frac{\alpha}{\Delta x} \begin{bmatrix} 1 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & -1 & 2 & -1 \\ & & & -1 & 1 \end{bmatrix} \{X\} = \lambda \frac{\Delta x}{6} \begin{bmatrix} 2 & 1 & & & \\ 1 & 4 & 1 & & \\ & 1 & 4 & 1 & \\ & & 1 & 2 & \\ & & & 1 & 2 \end{bmatrix} \{X\}$$

this matrix relationship is true for $\{X\} = \{u\}$ and $\lambda = 12\alpha/(\Delta x)^2$. Using Fried's theorem, (6.2), this eigenvalue is the maximum eigenvalue of the global system.

The maximum eigenvalue for the lumped system, (4.14), is

$$\lambda_n = 4\alpha/(\Delta x)^2$$

which gives the allowable time step for stable solutions as

$$\Delta t = \frac{(\Delta x)^2}{2\alpha(1-2\theta)} \quad (6.4)$$

Eq. (6.4) agrees with the lumped finite difference time step given by Lemmon (1969). Note that Δt for the lumped system is three times that of the consistently formulated system.

6.3 UNIFORM TWO-DIMENSIONAL GRIDS

The eigenvalue analysis for a pair of two-dimensional elements is summarized here. The two grids consist of: (i) square elements, and (ii) right triangular elements. The largest element eigenvalue for the consistent formulation and square element is $\lambda_n = 24D/\rho cA$. When substituted in (2.60), the stability restriction for Euler's method becomes

$$\alpha \Delta t / (\Delta x)^2 \leq 1/12 \quad (6.5)$$

which is identical to the result obtained using Von Neumann's method reported by Yalamanchili, (1973).

The element matrices (consistent formulation) for the element shown in Figure 6.1 are

$$[k^{(e)}] = \frac{D}{2} \begin{bmatrix} 1 & -1 & 0 \\ -1 & 2 & 1 \\ 0 & -1 & 1 \end{bmatrix} ; \text{ and } [C^{(e)}] = \frac{\rho cA}{12} \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix}$$

The largest eigenvalue of $[k^{(e)}]\{X\} = [c^{(e)}]\{X\}$ is

$$\lambda_n = \frac{18D}{\rho cA} \quad (6.6)$$

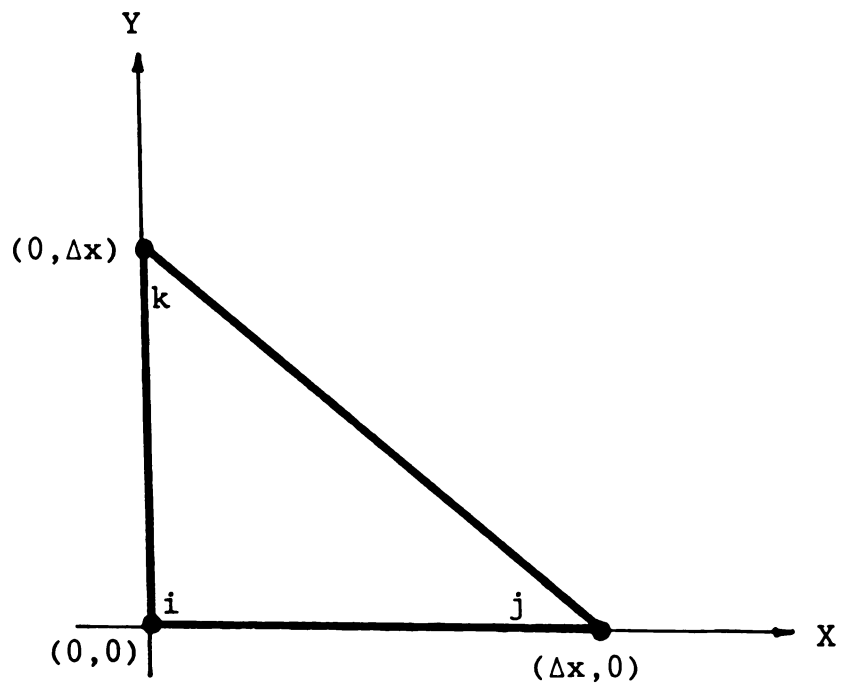


Figure 6.1 Right triangular element.

Using (2.60), the stability limit for Euler's technique is

$$\alpha \Delta t / (\Delta x)^2 \leq 1/18 \quad (6.7)$$

which agrees with a value given by Myers (1977).

An interesting fact comes from comparing (6.5) and (6.7). These two inequalities show that the square element has an allowable time step which is 50 percent larger than that for a right triangular element. Therefore, as far as the time step is concerned, the square element should never be divided into two triangular elements. The triangular element should only be used when it is necessary to model irregular boundaries.

6.4 NON-UNIFORM ONE-DIMENSIONAL GRID

To estimate the maximum time step that can be used in the numerical solution it is necessary to evaluate the largest eigenvalue of $[K]\{X\} = \lambda [C]\{X\}$. As discussed earlier this computation is expensive and impractical for a large system of equations. An estimate of λ_N can be used if it is relatively accurate.

The estimate reported in this study calculates the largest eigenvalue of a subregion which contains the elements with the largest element eigenvalue. Considering a subregion with a variable number of elements (one to ten), the largest eigenvalue of the subregion is λ_s . The ratio of λ_s to the eigenvalue of the whole system, λ_N , indicates how close the eigenvalue of the subsystem is to that of the

global system. When this ratio approaches unity, the sub-region can be used to estimate the time step value.

Table 6.1 is a summary of ten different one-dimensional grids used to develop the data points for the curve in Figure 6.2. Each grid contained ten elements. Some of the grids were uniform, some were non-uniform. Different types of boundary conditions were also considered. These consisted of specified temperatures, heat input and convection heat transfer.

Figure 6.2 is a plot of data in Table 6.1 to illustrate the idea mentioned above. The horizontal axis is the number of elements and the vertical axis shows the ratio of the subregion maximum eigenvalue to maximum eigenvalue of the complete system. When this ratio is close to one, the corresponding number of elements is all that must be analyzed to determine the largest eigenvalue. Figure 6.2 indicates that a subregion consisting of three elements is adequate for estimating the largest eigenvalue. For three elements, $\lambda_s/\lambda_N \approx 1.05$.

6.5 THE RADIAL ELEMENT

A two dimensional problem which has symmetry about a point can often be solved using the one-dimensional radial element shown in Figure 6.3.

Table 6.1:
One-dimensional grids used to calculate λ_s/λ_N .

Boundary Conditions	Grid		Coordinate System	Materials	
	Uniform	Non-Uniform	Cartesian	Radial	Single Composite
A. Temperature Specified at each end					
1.	X		X		X
2.		X	X		X
3.	X			X	X
4.	X		X		X
5.		X	X		X
B. Heat source at $x(0)$, insulated at $x(1)$					
6.		X	X		X
7.	X			X	X
8.		X		X	X
C. Insulated at $x(0)$, convection at $x(1)$					
9.		X	X		X
10.		X		X	X
Summary	4	6	6	4	8 2

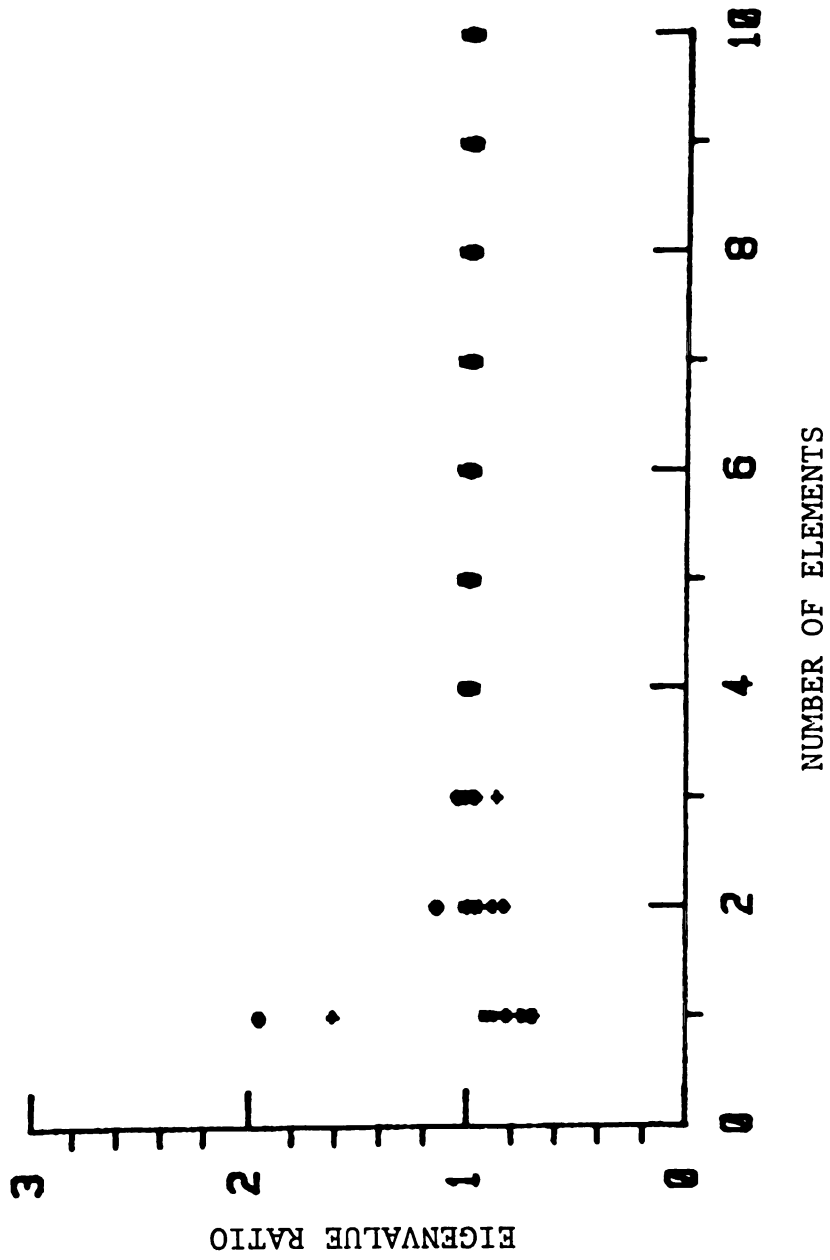


Figure 6.2 One-dimensional non-uniform grids.

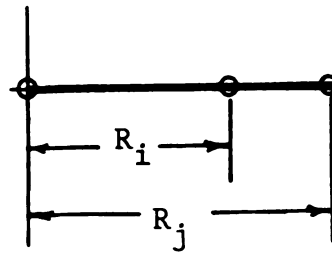
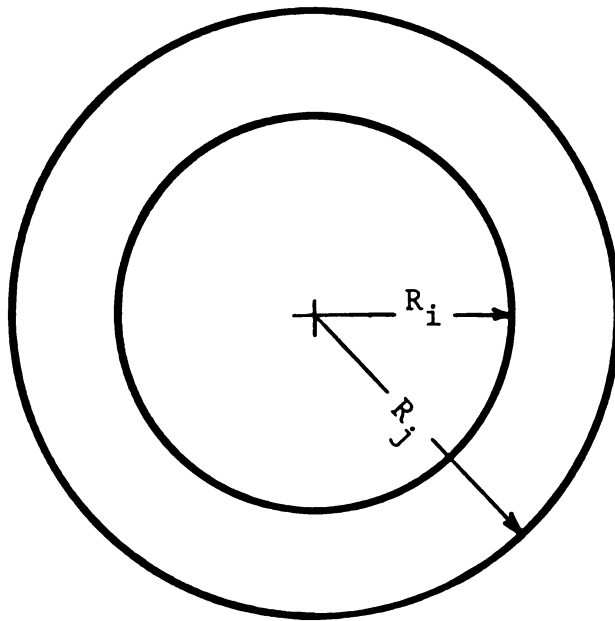


Figure 6.3 Linear radial element.

The element matrices for a radial element are, Segerlind (1976).

$$[k^{(e)}] = \frac{2 \pi K_r}{\Delta R} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \quad (6.8)$$

and

$$[C^{(e)}] = \frac{\pi \rho c \Delta R}{3} \begin{bmatrix} \bar{r} + R_i & \bar{r} \\ \bar{r} & \bar{r} + R_j \end{bmatrix} \quad (6.9)$$

for the consistent formulation and

$$[C^{(e)}] = \frac{\pi \rho c \Delta R}{3} \begin{bmatrix} 2\bar{r} + R_i & 0 \\ 0 & 2\bar{r} + R_j \end{bmatrix} \quad (6.10)$$

for the lumped formulation where $\bar{r} = (R_i + R_j)/2$. The thermal properties K_r , ρ and c are assumed constant and ΔR is the length of the element ($R_j - R_i$).

The estimation of allowable time step requires the computation of the largest eigenvalue of (6.1). Using the element matrices for the radial element gives

$$\frac{2\pi\bar{r}K_r}{\Delta R} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \{X\} = \lambda \frac{\pi\rho c(\Delta R)}{3} \begin{bmatrix} \bar{r} + R_i & \bar{r} \\ \bar{r} & \bar{r} + R_j \end{bmatrix} \quad (6.11)$$

from which the eigenvalues are

$$\lambda_1 = 0$$

and

$$\lambda_2 = \frac{36K_r \bar{r}^2}{\rho c (2\bar{r}^2 + R_i R_j) (\Delta R)^2}$$

For large values of R_i and small element length, R , the approximate value of λ_2 is

$$\lambda_2 \approx \frac{12K_r}{\rho c (\Delta R)^2} \approx \frac{12\alpha}{(\Delta x)^2} \quad (6.12)$$

which is the same as obtained for the linear case in cartesian coordinates. The analysis for the lumped cases is similar and the largest eigenvalue is

$$\lambda \approx \frac{4\alpha}{(\Delta R)^2} \quad (6.13)$$

which is the value for lumped formulation in one-dimensional cartesian linear element.

For small values of R_i , the elements have eigenvalues different from those in (6.12) and (6.13) and the problem should be treated as a non-uniform grid.

6.6 TWO-DIMENSIONAL GRIDS

The analysis of some two-dimensional grids using the subregion idea are presented in this section. Eight different triangular grids with different element size and shapes and different boundary conditions were used for this study. One of the non-uniform grids with insulated boundaries is shown in Figure 6.4. Since the smallest elements

have maximum eigenvalues, the subregion in the lower left corner were combined to form subregions and λ_s was calculated for each subregion.

Table 6.2 contains a partial description of all eight grids and the corresponding eigenvalue ratio with respect to element number has been plotted in Figure 6.5. The results are similar to those for the one-dimensional grids. A subregion consisting of the five smallest elements gives a satisfactory estimate of the largest eigenvalue. For five elements, $\lambda_s/\lambda_N \approx 1.05$.

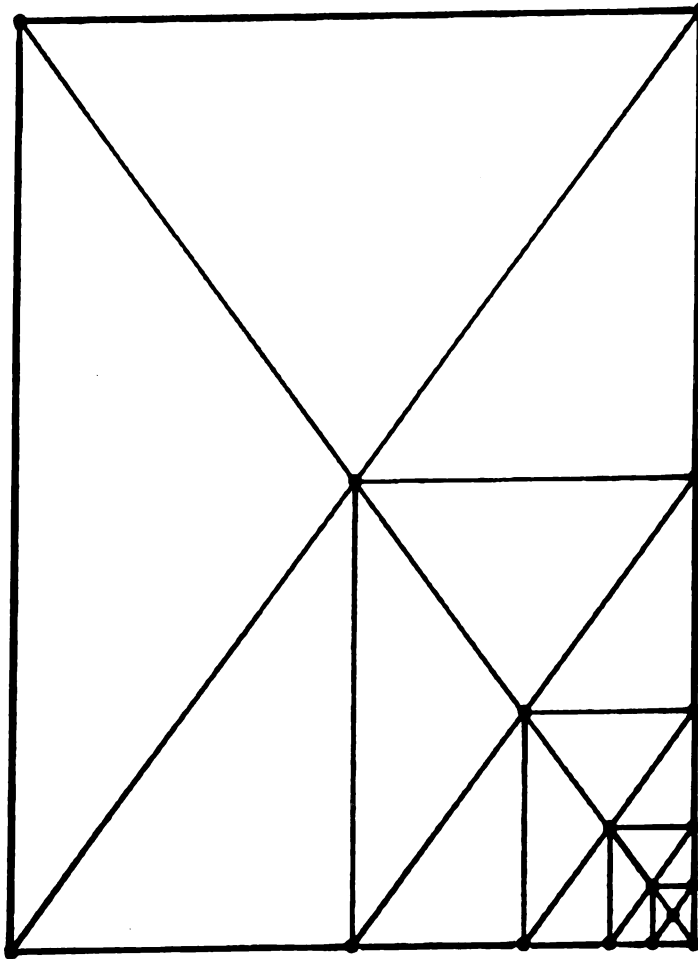


Figure 6.4 Unequal triangular gird.

Table 6.2:
Two-dimensional grids used to calculate λ_s/λ_N

Boundary Conditions	Grid		Single Material
	Uniform	Non-Uniform	
A. Insulated boundaries and Heat source at first node			
1.	X		X
2.		X	X
3.		X	X
4.		X	X
5.		X	X
6.		X	X
B. Convective Boundary Conditions			
7.	X		X
8.		X	X
Summary	2	6	8

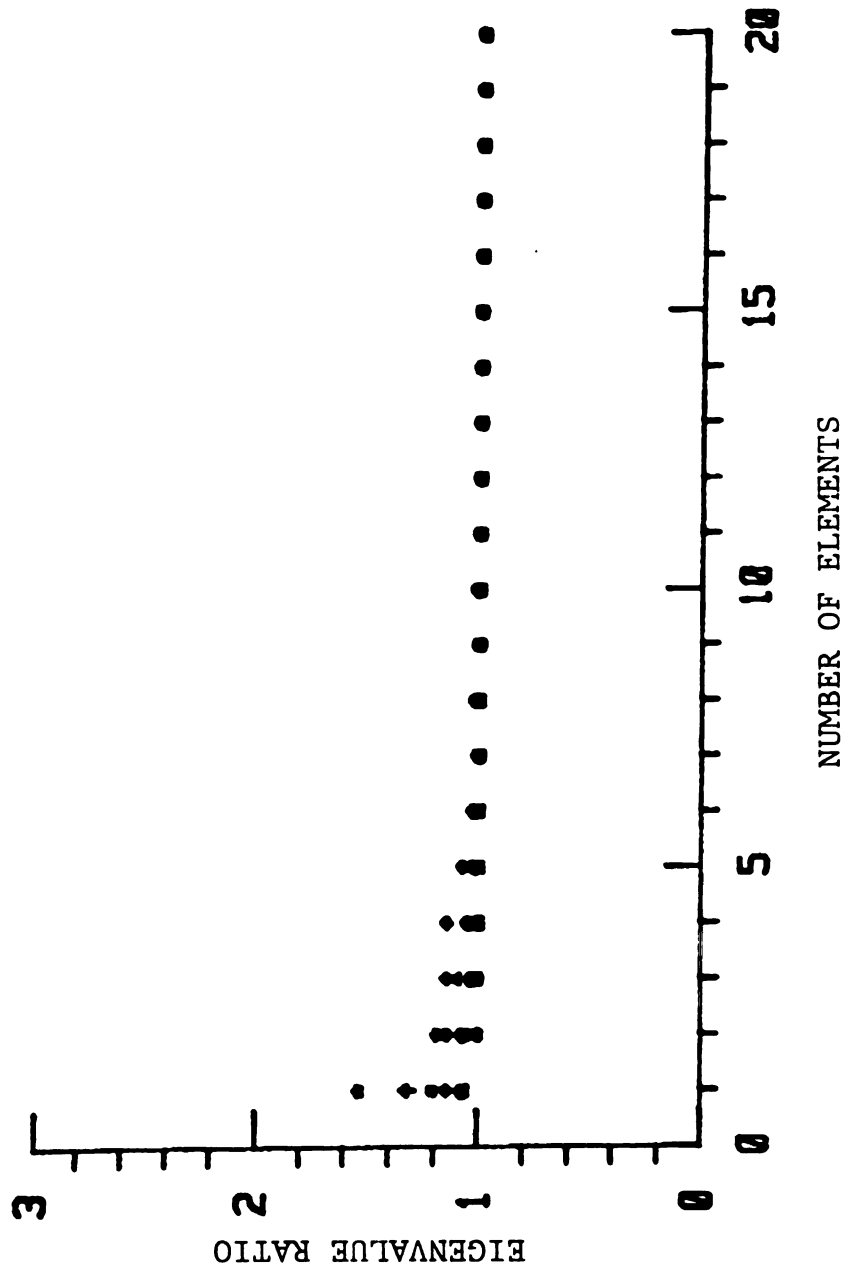


Figure 6.5 Two-dimensional non-uniform grids.

CHAPTER VII

CONCLUSIONS

The objective of this study was to investigate the numerical difficulties associated with the solution of transient field problems. This study consisted of four parts; establishment of the necessary properties for $[A]$ and $[P]$ in $[A] \{T\}_{n+1} = [P]\{T\}_n$, investigation of the consistent and lumped formulations, a study of individual elements and an estimation of the maximum time step which can be used and still avoid numerical oscillations.

Specific conclusions from this study include:

1. The following properties are required for matrices $[A]$ and $[P]$ in order to meet Positive Coefficient Rules:
(i) $[A]$ must have positive diagonals and negative off-diagonal entries, (ii) $[P]$ must be positive definite with positive entries.
2. The maximum allowable integration time step for the consistent finite element formulation is small compared to the lumped formulations. For example, in one dimensional (linear) uniform grids the time step for the lumped formulation is three times that for the consistent formulation.
3. It is very difficult to meet Positive Coefficient Criteria using the consistent formulation.

4. The positive Coefficient Criteria requires the convection part of the stiffness matrix to be lumped.

5. The analytical solution of the temperature distribution in an insulated rod showed that the lumped formulations gave results which are physically realistic while the consistent formulation gave unrealistic values for small values of time.

6. The interior angles of triangular elements should be less than or equal to 90° .

7. The aspect ratio for rectangular elements should not exceed by $\sqrt{2}$.

8. The one- and two-dimensional quadratic elements fail to meet the Positive Coefficient Rule.

9. Division of a square into two right triangles decreases the allowable time step value by a factor of 1.5.

10. The maximum eigenvalue of a subregion consisting of the five smallest elements in a grid yields a good estimate for the time step.

11. The uniform radial elements (equal ΔR) can be treated as a uniform grid.

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