NONLINEAR HEAT TRANSFER AND THERMO/MECHANICAL STRESS ANALYSIS USING FINITE ELEMENTS

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I, Derek Steven Pennington submit this thesis in partial fulfilment of the requirements for the degree of Master of Science in Engineering. I claim that this is my original work and that it has not been submitted in this or similar form for a degree at any University.

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ABSTRACT

This thesis deals with the development, implementation and testing of numerical procedures for the heat transfer and thermo-mechanical analysis of solid continua. Steady state conduction heat transfer is developed as a particular case of the general field equation. Internal heat generation and the boundary conditions of specified temperatures, flux, convection, and radiation are included. The stress - strain - temperature relationships for a corresponding body are not coupled to the heat transfer relationships for steady state conditions. The heat transfer problem is thus solved prior to, and independently of, the mechanical problem. The resulting temperature field is adopted for the solution of the thermal deformation problem. Finite element formulations using a common discretization are developed for these problems using Galerkin's method. The formulations are implemented in an existing temperature independent nonlinear finite element stress analysis code. Four, eight and nine noded isoparametric continuum finite elements with the option of the plane stress, plane strain and axisymetric cases are utilized. Nonlinear heat transfer due to temperature dependent thermal conductivity and/or internal heat generation is solved using an iterative method based on the Newton-Raphson algorithm. Thermal deformations and stresses are determined by calculating equivalent nodal loads corresponding to the thermal strains which result from the temperature field. These are then applied to the mechanical model. The implementation is illustrated by three examples whose solutions compare favourably with analytical solutions taken from the literature.

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NOMENCLATURE

Upper case characters

E - Young's modulus

G - shear modulus

J - Jacobian

M - number of elements in domain

N - interpolation function

P - point source

Q - internal heat generation

R_q - edge flux

T - temperature

W - numerical integration weighting factors

Lower case characters

a,b - constants to define a linear conductivity/ temperature relationship

h - convection heat transfer coefficient

i,j - counters

k - conductivity

m - total number of nodes in domain

n - number of nodes per element

$n_{x,y,z}$ - direction cosines of surface outward normal

r - r^{th} node of element with n nodes.

t - element thickness

Superscripts

$( )^{(e)}$ - element designation

$( )^{T}$ - matrix transpose

Subscripts

$(\ )_{ij}$ - numerical integration counters

$(\ )_{xyz}$ - cartesian components

$(\ )_{rz\theta}$ - cylindrical components

$T_{e,o}$ - exchange and reference temperatures respectively

$(\ )_{1,2,\ldots,r,\ldots,n}$ - nodes 1 through r to n

$\Gamma_{hpqRTtu}$ - surfaces with specified convection, point sources, flux, radiation, temperatures, tractions and displacements respectively.

Vectors

{a} - general nodal displacements

{d} - cartezian partial derivatives for a vector

{F} - nodal loads

{g} - temperature gradients

{L} - thermal strain equivalent loads

{n} - surface outward normal

{P} - thermal expansions

{q} - heat flux

{R} - nodal fluxes

{T} - nodal temperatures

{t} - surface traction

{u} - prescribed displacement

{w} - arbitrary displacement field

$\{\delta\}$ - cartezian partial derivatives for a scalar

$\{\epsilon\}$ - strains

$\{\sigma\}$ - stress

Matrices

[B] - gradient interpolation matrix
[C] - conductance matrix
[D] - elasticity matrix
[J] - Jacobian matrix
[K] - stiffness matrix
[k] - conductivity tensor
[N] - general interpolation matrix
[S] - residual flux matrix

Special symbols

∂ - partial derivative
∇^2 - Laplacian operator

Greek characters

α - coefficient of thermal expansion
Γ - domain boundary
γ_{ij} - shear strain
ϵ_{ij} - normal strain components
ϵ - surface emissivity
ξ,η - natural coordinates for isoparametric elements
κ - surface absorptivity
μ,ρ - field equation constants
ν - Poissons ratio
σ - Stefan Boltzmann constant
σ_{ij} - normal stress components
τ_{ij} - shear stress components
ϕ - field variable
Ω - solution domain

CHAPTER ONE

INTRODUCTION

The finite element method has established itself in engineering as a powerful tool for the stress analysis of complex structural systems. Some of the most challenging applications of the method are in areas where the mechanical stress problem interacts with other physical phenomena.

One such application is the behaviour of solids under temperature changes. In such cases the determination of temperatures by conduction heat transfer for practical structures often requires the consideration of several temperature dependent parameters such as thermal conductivity and internal heat generation. This constitutes a nonlinear problem. Depending on the state of stress in the material, any deformation might also be nonlinear.

This thesis sets out to develop finite element formulations for nonlinear conduction heat transfer and thermo-mechanical stress analysis.

The theory is implemented in the specialized but temperature independent code, NOSTRUM[1], (NOnlinear STRUctural Mechanics) which has been developed by the UCT/CSIR Applied Mechanics Research Unit at the University of Cape Town. The ability for both conduction heat transfer and thermo-mechanical analysis is implemented for plane finite continuum elements so that a single discretization may be used for either type of analysis.

While the thermo-mechanical aspect only required adjustment of existing stress analysis procedures in NOSTRUM, the entire heat transfer aspect had to be developed and implemented. Consequently greater detail is devoted to the latter.

1.1 INTRODUCTION TO FIELD PROBLEMS

Heat conduction belongs to a group of physical field problems which are governed by transient, nonlinear quasi-harmonic partial differential equations. These equations have the form

$$\frac{\partial}{\partial x}(k_x\frac{\partial \phi}{\partial x}) + \frac{\partial}{\partial y}(k_y\frac{\partial \phi}{\partial y}) + \frac{\partial}{\partial z}(k_z\frac{\partial \phi}{\partial z}) + Q - \mu\frac{\partial \phi}{\partial t} - \rho\frac{\partial^2 \phi}{\partial t^2} = 0 \quad (1.1)$$

where $\phi = \phi(x,y,z,t)$ is an unknown scalar field,
$Q = Q(x,y,z,t,\phi)$ is a source term,
and k_x, k_y, k_z, μ, ρ are physical coefficients which may vary with space and time, and with ϕ or its derivatives.

Typical examplcs are transient heat conduction, wave transmission in fluids and the diffusion of a chemical species from a region of high concentration to a region of low concentration.

The time dimension is included for various problems in texts by Zienkiewicz[2], Rao[3] and Heubner[4], but in this thesis all analysis is considered to be steady state.

1.2 STEADY STATE FIELD PROBLEMS

The steady state form of the field equation is obtained by reducing equation 1.1 to:

$$\frac{\partial}{\partial x}(k_x\frac{\partial \phi}{\partial x}) + \frac{\partial}{\partial y}(k_y\frac{\partial \phi}{\partial y}) + \frac{\partial}{\partial z}(k_z\frac{\partial \phi}{\partial z}) + Q = 0 \quad (1.2)$$

Examples of steady state field problems governed by this equation are listed in table 1.1

FIELD PROBLEM	SCALAR FIELD ϕ	k_x, k_y, k_z	SOURCE Q
Heat conduction	Temperature	Thermal conductivity	Internal heat generation
Torsion	Stress function	(Shear modulus)$^{-1}$	Twist per unit length
Diffusion	Concentration	Diffusivity	-
Seepage	Pressure	Permeability	Internal flow source
Magnetostatics	Magneto force	Magnet permeability	Internal magnetic field source
Reynolds film lubrication	Pressure	(film thickness) / viscosity	Lubricant supply
Bingham plastic flow	Velocity potential	Viscosity	Pressure gradient
Electric conduction	Voltage	Electric conductivity	Internal current source
Compressible flow	Velocity potential	Density	-

Table 1.1 Physical situations governed by the quasi-harmonic steady state equation.

The description of such field problems is not complete until relevant boundary conditions are applied.

Consider the field variable ϕ to be defined in a general three dimensional solution domain, Ω, bounded by a surface, Γ, (Figure 1.1).

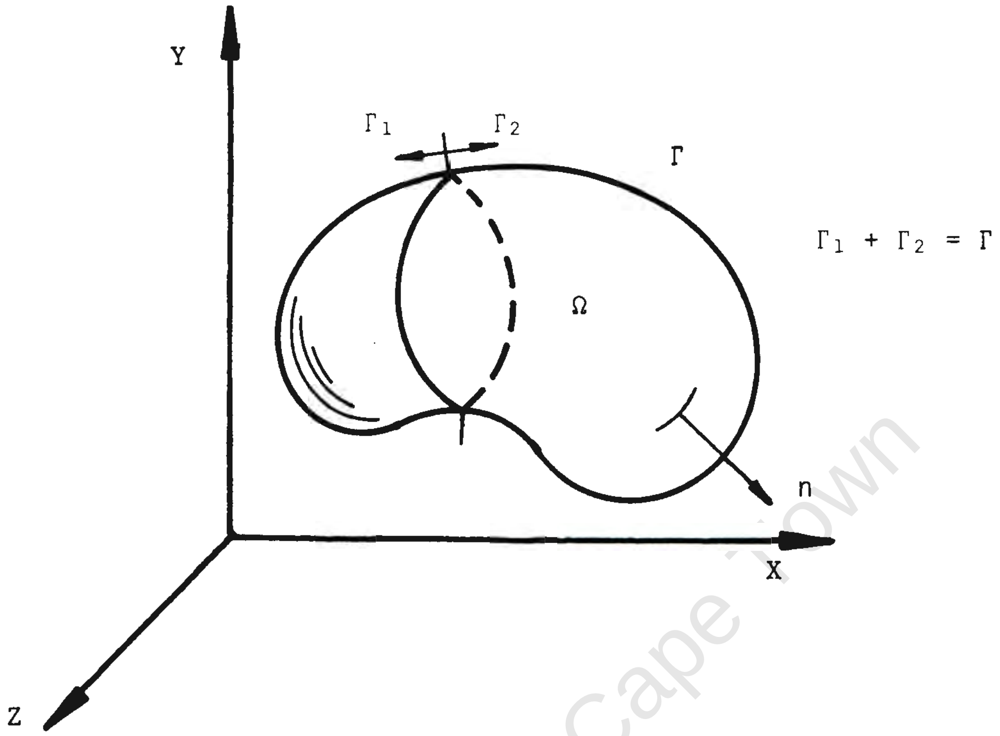


Figure 1.1 Three dimensional solution domain

Referring to Figure 1.1, the two main types of boundary conditions considered are:

a) The value of the field variable specified on part (or whole) of the boundary, Γ_1

$$\phi = \phi(x,y,z) \tag{1.3}$$

b) On the remaining part of the boundary, Γ_2, the Cauchy or "natural" boundary condition is

$$k_x \frac{\partial \phi}{\partial x} n_x + k_y \frac{\partial \phi}{\partial y} n_y + k_z \frac{\partial \phi}{\partial z} n_z + q(x,y,z,\phi) - h(x,y,z,\phi)\phi = 0 \tag{1.4}$$

where q and h can be functions of both position and the field variable, and n_x, n_y and n_z are the direction cosines of the outward normal to the surface.

If the body is isotropic, ie $k_x = k_y = k_z = k$ = constant, the general formulation given by equations 1.2, 1.3, and 1.4 can be reduced to give Poisson's equation,

$$\nabla^2 \phi = \frac{Q}{k} \qquad (1.5)$$

If there are no source terms, ie Q = 0, equation 1.5 can be further reduced to give the well known Laplace equation

$$\nabla^2 \phi = 0 \qquad (1.6)$$

1.3 CLOSURE

The theory and finite element formulation of conduction heat transfer and thermo-mechanical stress analysis are described in Chapter Two.

Chapter Three deals with the implementation of the formulations into NOSTRUM. The calculation procedures required for isoparametric elements are given.

The theory is illustrated in Chapter Four by three examples which are compared with published analytical solutions.

The thesis ends with conclusions and recommendations in Chapter Five.

CHAPTER TWO

DEVELOPMENT OF THEORY

2.1 HEAT TRANSFER

2.1.1 Steady State Heat Conduction

The solution domains for the thermo-mechanical stress analysis techniques developed in this thesis are solid continua. The specific field problem is therefore conduction heat transfer, although convection and radiation on the boundaries of the domain are included.

Consider steady state heat transfer in a three dimensional anisotropic solid Ω bounded by a surface Γ (Figure 2.1)

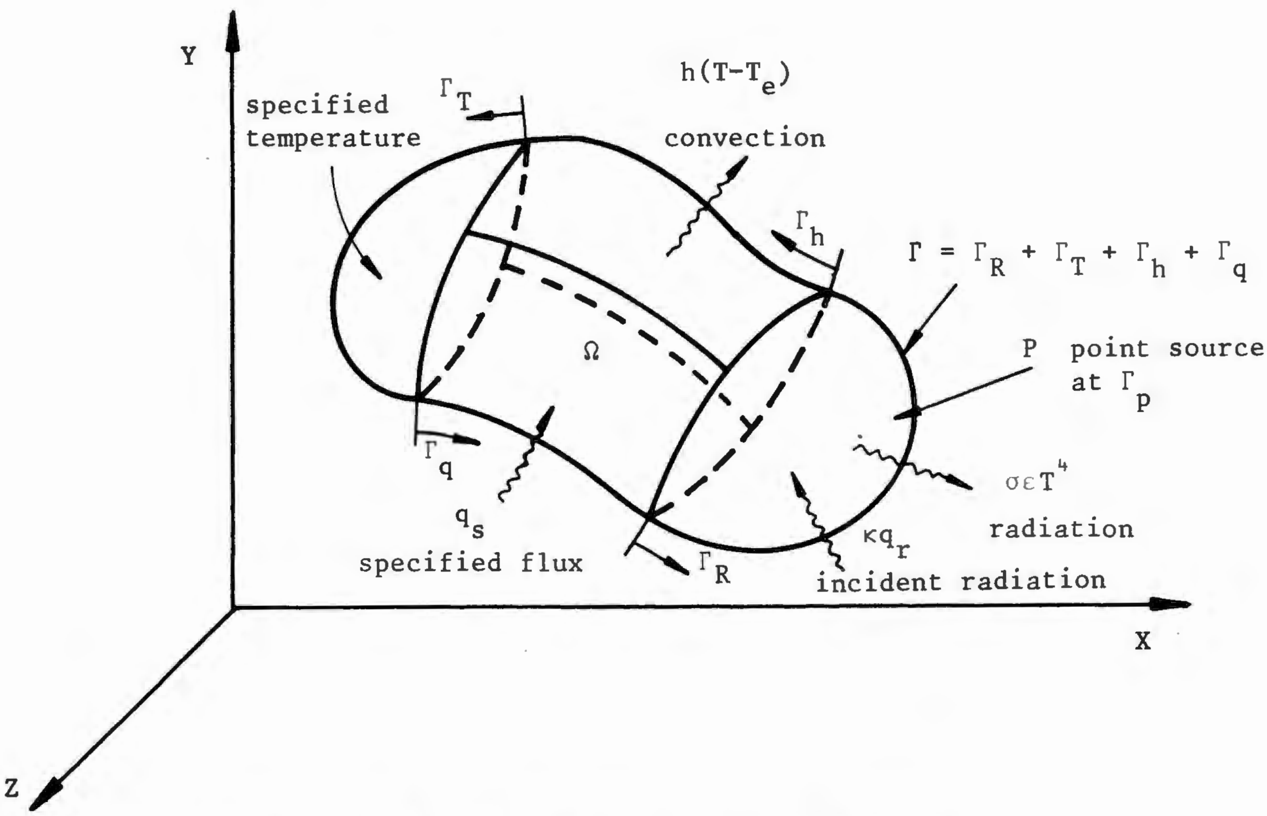


Figure 2.1 Three dimensional solution domain for general heat conduction

For the system to satisfy conservation of energy, the following balance must exist.

Heat inflow + Heat generated internally = Heat outflow + Change in internal energy

This balance leads to the energy equation

$$-\left(\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z}\right) + Q = 0 \qquad (2.1)$$

where q_x, q_y and q_z correspond to heat flux in the cartesian directions and $Q=Q(x,y,z,t)$ is the internal heat generation.

The rate equation describing heat conduction is Fourier's law, which for an anisotropic medium is

$$\{q\} = -[k]\{g\} \qquad (2.2)$$

where $\{q\} = [q_x \;\; q_y \;\; q_z]^T$ – heat flux vector

$$[k] = \begin{bmatrix} k_{11} & k_{12} & k_{13} \\ k_{21} & k_{22} & k_{23} \\ k_{31} & k_{32} & k_{33} \end{bmatrix}$$ – conductivity maxtrix

$$\{g\} = \left[\frac{\partial T}{\partial x} \;\; \frac{\partial T}{\partial y} \;\; \frac{\partial T}{\partial z}\right]^T$$ – temperature gradient vector

Substitution of equation 2.2 into the energy equation 2.1 gives the general field equation with temperature as the field variable. In matrix notation this is

$$\{\delta\}^T[k]\{g\} + Q = 0 \qquad (2.3)$$

where $\{\delta\}^T = \left[\frac{\partial}{\partial y} \;\; \frac{\partial}{\partial x} \;\; \frac{\partial}{\partial z}\right]$

The general boundary conditions given in equations 1.3 and 1.4, are expanded to include the boundary conditions for conduction shown in figure 2.1, to give

1) A prescribed temperature on Γ_T

$$T_T = T(x, y, z) \tag{2.4a}$$

2) A specified flux on Γ_q

$$\{q\}^T \{n\} = q_s \tag{2.4b}$$

where $\{n\} = [n_x \ n_y \ n_z]^T$ are the direction cosines of the outward normal to the surface.

3) A convective exchange flux on Γ_h

$$\{q\}^T \{n\} = -h(T - T_e) \tag{2.4c}$$

where h is a convective heat transfer coefficient, T is the surface temperature and T_e is the surrounding or exchange temperature

4) A radiation flux transfer on Γ_R

$$\{q\}^T \{n\} = \sigma\epsilon T^4 - \kappa\ q_r \tag{2.4d}$$

where σ is the Stefan-Boltzmann constant, ϵ is the surface emissivity, κ is the surface absorptivity and q_r is the incident radiant heat flow per unit area.

5) A concentrated source at the point Γ_p

$$\{q\}^T \{n\} = -P \tag{2.4e}$$

Expressed in these terms the boundary conditions now include the inherently nonlinear convection and radiation boundary conditions.

There are three fundamental approaches traditionally used to generate finite element formulations to the heat conduction problem.

Oden[5] gives a generalised interpretation of finite element equations showing how they can be developed from well established global energy balances. For a region that has already been discretized he states, "all that is needed is some means to translate a relation that holds at a point (in the solution domain) into one that must hold over a finite region". This first approach is termed the "energy balance" or "physical" approach which Wilson[6] and Oden [7] show to provide additional insight into some solution processes.

Secondly, in the classical variational approach finite element equations are obtained by minimising a discretized functional of the problem expressed in terms of the discrete nodal temperatures. Thirdly, regarding the Galerkin approach using weighted residuals, Huebner[4] states that Galerkin's method "not only encompasses the variational approach but also goes far beyond, because it can be applied to any well posed system of differential equations and their boundary conditions".

This method is used in the next section to develop a finite element formulation, as it lends itself neatly to both the thermal and stress problems.

2.1.2 Finite Element Formulation

The solution domain Ω is divided into M elements of n nodes each, and a general interpolation matrix [N] consisting of n shape function is specified for an element:

$$[N] = [N_1 , N_2 \, ... N_n] \tag{2.5a}$$

The corresponding gradient interpolation matrix [B], is

$$[B] = \begin{bmatrix} \frac{\partial N_1}{\partial x} & \frac{\partial N_2}{\partial x} & \cdots\cdots & \frac{\partial N_n}{\partial x} \\ \frac{\partial N_1}{\partial y} & \frac{\partial N_2}{\partial y} & \cdots\cdots & \frac{\partial N_n}{\partial y} \\ \frac{\partial N_1}{\partial z} & \frac{\partial N_2}{\partial z} & \cdots\cdots & \frac{\partial N_n}{\partial z} \end{bmatrix} \qquad (2.5b)$$

The temperature at any point in an element can now be approximated in terms of the interpolation functions by

$$T^{(e)}(x,y,z) = [N(x,y,z)]\{T\} \qquad (2.5c)$$

where {T} is the vector of nodal temperatures. Similarly, temperature gradients within an element can be expressed by

$$\left\{ \begin{matrix} \frac{\partial T}{\partial x}(x,y,z) \\ \frac{\partial T}{\partial y}(x,y,z) \\ \frac{\partial T}{\partial z}(x,y,z) \end{matrix} \right\} = [B(x,y,z)]\{T\} \qquad (2.5d)$$

The second order heat conduction equation requires C^0 continuity, and temperature is the only nodal unknown. Focusing on a single element, the Galerkin method is used to derive the finite element equations. Starting with the energy equation 2.1 for a single element, the method requires that

$$\int_{\Omega^{(e)}} \left(\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z} - Q\right) N_r \, d\Omega = 0 \qquad (2.6)$$

where $\Omega^{(e)}$ is the element domain.

This indicates that the error or residual introduced by the approximation on the left hand side is required to vanish in an average sense over the domain.

The term

$$\int_{\Omega^{(e)}} \left(\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z}\right) N_r \, d\Omega$$

is integrated using Gauss's theorem to introduce the heat flow across the element boundary $\Gamma^{(e)}$.

The result is

$$-\int_{\Omega^{(e)}} \left(q_x \frac{\partial N_r}{\partial x} + q_y \frac{\partial N_r}{\partial y} + q_z \frac{\partial N_r}{\partial z}\right) d\Omega = \int_{\Omega^{(e)}} N_r Q \, d\Omega$$

$$+ \int_{\Gamma^{(e)}} (q_x n_x + q_y n_y + q_z n_z) N_r \, d\Gamma \qquad r = 1,2,\ldots n \qquad (2.7)$$

The surface integral in equation 2.7 allows for the introduction of the natural boundary conditions (equations 2.4 a-e) to give

$$-\int_{\Omega} \left[\frac{\partial N_r}{\partial x}, \frac{\partial N_r}{\partial y}, \frac{\partial N_r}{\partial z}\right] \{q\} \, d\Omega = \int_{\Omega} Q N_r \, d\Omega - \int_{\Gamma_T} \{q\}^T \{n\} N_r \, d\Gamma$$

$$+ \int_{\Gamma_q} q_s N_r \, d\Gamma - \int_{\Gamma_h} h(T-T_e) N_r \, d\Gamma - \int_{\Gamma_R} (\sigma \epsilon T^4 - \kappa q_r) N_r \, d\Gamma + P_r \quad (2.8)$$

where for simplicity Ω now refers to the element area $\Omega^{(e)}$ and $\Gamma_{(\ )}$ refers to that part of the element boundary $\Gamma^{(e)}$ where one of the specific boundary conditions exists.

Fourier's law (equation 2.2) can be written in terms of the element temperature gradients as

$$\{q\} = -[k]\,[B]\,\{T\} \qquad (2.9)$$

Introducing equation 2.9 and the element temperatures to equation 2.8, the resulting element equations are:

$$\int_{\Omega} [B]^T[k][B]\{T\}\, d\Omega = \int_{\Omega} Q[N]^T\, d\Omega - \int_{\Gamma_T} \{q\}^T\{n\}[N]^T d\Gamma$$

$$+ \int_{\Gamma_q} q_s[N]^T d\Gamma - \int_{\Gamma_h} h[N]^T[N]\{T\} - hT_s[N]^T\, d\Gamma +$$

$$\int_{\Gamma_R} (\sigma\epsilon[N]^T[N]\{T\}[N]\{T\}[N]\{T\}[N]\{T\} - \kappa q_r[N]^T)d\Gamma + \{P\} \quad (2.10)$$

A conductance matrix, [C], and a flux vector {R}, are now defined so that equation 2.10 can be written as:

$$[[C_c]+[C_h]+[C_R]]\{T\}=\{R_T\}+\{R_Q\}+\{R_q\}+\{R_h\}+\{R_R\}+\{R_p\} \quad (2.11)$$

where the conductance matrix components are

$[C_c] = \int_{\Omega} [B]^T[k][B]d\Omega$ - Conductivity matrix

$[C_h] = \int_{\Gamma_h} h[N]^T[N]d\Gamma$ - Convection matrix

$[C_R]\{T\} = \int_{\Gamma_R} \sigma\epsilon[N]^T[N]\{T\}[N]\{T\}[N]\{T\}[N]\{T\}d\Gamma$ - Radiation matrix

and the flux vector components are

$\{R_T\} = \int_{\Gamma_T} \{q\}^T\{n\}[N]^T d\Gamma$ - Reaction flux vector

$\{R_Q\} = \int_{\Omega} Q[N]^T d\Omega$ - Internal heat generation vector

$\{R_q\} = \int_{\Gamma_q} q_s[N]^T d\Gamma$ - Surface flux vector

$\{R_h\} = \int_{\Gamma_h} hT_s[N]^T d\Gamma$ - Convective flux vector

$\{R_R\} = \int_{\Gamma_R} \kappa q_r [N]^T d\Gamma$ — Incident radiation flux vector

$\{R_p\} = P_r \quad r = 1,2,\ldots.n$ — Vector of point sources

Note that $\{R_T\}$ are unknown flux distributions on boundary Γ_T where temperatures are prescribed. They are only computed once the temperature field has been determined and are the heat flux reactions necessary to maintain the nodes on Γ_T at their specified temperatures.

Equation 2.11 is the general nonlinear finite of element equation for conduction in an anistropic solid medium. Assembly of the element equations to obtain the global system of equations follows the standard procedure of summing all elements to form an m x m conductance matrix, where m is the total number of nodes. Since the heat transfer elements developed in this thesis are to be used in conjunction with displacement/stress elements, it is important to note that the field variable temperature, is a scalar quantity. This means that transformations of matrices computed in local coordinates systems are not necessary in order to form the global matrix.

The general equation 2.11 is often reduced for practical heat transfer cases to the linear equation

$$[[C_c]+[C_h]]\{T\} = \{R_Q\}+\{R_q\}+\{R_h\}+\{R_p\} \qquad (2.12)$$

by excluding radiation and assuming that [k], the conductivity, h the convection coefficient and Q, the internal heat generation, do not depend on temperature.

When material properties and their environments are significantly dependent on the temperature, the full nonlinear steady state equation to be solved is

$$[[C_c(T)] + [C_h(T)] + [C_R(T)]]\{T\} = \{R_Q(T)\} + \{R_q(T)\} + \{R_h(T)\} + \{R_R(T)\} + \{R_p(T)\} \qquad (2.13)$$

Solution techniques have discussed in a number of papers. Meric[8], Leelamma Mani[9] and Lyness[10] consider the conductivity to be isotropic and to vary linearly with temperature: ie k is of the form $k = k_o(1+aT)$ where k_o is the reference conductivity and "a" is a constant. Lyness[10] compares his finite element solution to a nonlinear problem of this type favourably with a variational formulation solution by Hays[11] .

Padovan[12] generalizes the finite element formulation for fully anisotropic media with $k_{ij} = k_{oij}(1+aT)$. Bathe[13] and Wilson[7] have examples demonstrating nonlinearities due to both linear variation of conductivity with temperature and the nonlinear convection boundary condition.

A recent paper by Reddy[14] on the conduction problem of a steel casting with both radiation and convection boundary conditions shows the importance of considering the highly nonlinear radiation boundary conditions present in metallurgical processes where this mode of heat transfer is significant.

Thornton[15] demonstrates the abilities of the method in considering the transient problem of a hydrogen cooled supersonic ramjet strut. The strut is heated on one side by hot hydrogen flowing in an internal manifold and on the other aerodynamically by external air flow. It is cooled by cold hydrogen flowing between the primary structure and the outer skin. This entails temperature dependent convection coefficients, thermal conductivity and specific heat. An aspect of that paper which is incorporated in this thesis is the piecewise continuous approximation of these properties. This aspect is discussed in Chapter 3.

A further topic of research related to nonlinear heat transfer is the type of equation solution algorithm used. Hughes[16] discusses a range of algorithms with respect to their stability. The most commonly used algorithm is the Newton-Raphson method, although it is not always the most efficient. Lyness[10] uses an iterative method which is based on the Newton-Raphson algorithm. In a sample problem where conductivity was assumed to vary linearly with temperature, this algorithm produced convergence in only one more iteration than the Newton-Raphson method. This being the case, and because of its simplicity relative to the full Newton-Raphson method, this iterative method is used in this thesis. The numerical implementation is discussed in Chapter 3.

2.2. THERMO-MECHANICAL STRESS ANALYSIS

2.2.1. Introduction

It is well known that changes in temperature cause bodies to deform. Uniform heating of an unconstrained isotropic body produces uniform stress free expansion of the material with no resultant stresses. Mechanical deformation occurs if a thermal gradient exists, or the body is mechanically restrained in one or more directions, or the material has an anisotropic coefficient of expansion. If this deformation occurs in the range of linear material response, the behaviour is governed by the equations of thermo-elasticity. In cases such as the solidification or heat treatment of metals, thermal deformation is often nonlinear.

In transient problems, thermo-elasticity is essentially a coupled problem of the heat transfer and mechanical deformation procedures. This requires a complete energy balance approach which is discussed by Biot[17]. In that paper the expression for the free energy developed for thermo-elasticity is referred to as a thermo-elastic potential and this leads to a variational formulation with a minimum entropy production principle. Keramidas[18][19] uses a similar variational formulation to produce a finite element formulation of the coupled thermo-mechanical problem.

However, many engineering text books neglect this coupling for general steady state problems. Zudans[20] in his text for the nuclear industry states that "The mechanical energy associated with deformation of the solid is usually neglected in reaching the energy balance". This is the approach taken in this thesis where in addition the solution region is assumed to have isotropic mechanical properties.

2.2.2. Stress-Strain-Temperature Relations

Thermo-elastic strain can be considered as consisting of two parts. One component is related to mechanical deformation by Hooke's Law and another results from free thermal expansion. Mechanical restraint or loading conditions are superimposed on the thermal expansion to give the general equations

$$\begin{aligned}
\epsilon_x &= \frac{1}{E}[\sigma_x - \nu(\sigma_y + \sigma_z)] + \alpha(T - T_0) \\
\epsilon_y &= \frac{1}{E}[\sigma_y - \nu(\sigma_x + \sigma_z)] + \alpha(T - T_0) \\
\epsilon_z &= \frac{1}{E}[\sigma_z - \nu(\sigma_x + \sigma_y)] + \alpha(T - T_0) \qquad (2.14) \\
\gamma_{xy} &= \frac{1}{G} \tau_{xy} \\
\gamma_{yz} &= \frac{1}{G} \tau_{yz} \\
\gamma_{zx} &= \frac{1}{G} \tau_{zx}
\end{aligned}$$

where E is Youngs modulus

ν is Poissons ratio

$G = E/(2(1+\nu))$ is the shear modulus

is the coefficient of isotropic expansion

T is the temperature

and T_0 is the reference temperature

From this point the relations are developed for plane two-dimensional cases. This enables the identification of the specific plane stress, plane strain and axisymmetric concepts which are used in the application of this theory.

Solving for the stresses, equations 2.14 reduce to the constitutive equation

$$\{\sigma\} = [D]\{\epsilon\} - [D]\{P\}\ (T-T_0) \qquad (2.15)$$

where $\{\sigma\} = [\sigma_x \ \ \sigma_y \ \ \tau_{xy}]^T$

and $\{\epsilon\} = [\epsilon_x \ \ \epsilon_y \ \ \gamma_{xy}]^T$

For plane stress where the stress component (σ_z) perpendicular to the plane must be zero

$$[D] = \frac{E}{1-\nu^2}\begin{bmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & (1-\nu)/2 \end{bmatrix}$$ – elasticity matrix

and $\{P\} = \alpha\ [1 \ \ 1 \ \ 0]^T$ – Thermal expansion vector

For plane strain where the perpendicular stress component (σ_z) is non-zero, but the corresponding strain component (ϵ_z) is zero

$$[D] = \frac{E}{(1+\nu)(1-2\nu)}\begin{bmatrix} 1-\nu & \nu & 0 \\ \nu & 1-\nu & 0 \\ 0 & 0 & (1-2\nu)/2 \end{bmatrix}$$

and $\{P\} = (1+\nu)\alpha\ [\ 1 \ \ 1 \ \ 0\ ]^T$

and the stress in the direction perpendicular to the plane due to thermal expansion is

$$\sigma_z = -E\alpha(T - T_o)$$

For the axisymetric case where the x direction of the previous cases corresponds to the radial component, and the y direction to the axis of symmetrical rotation.

$$\{\sigma\} = [\sigma_r \quad \sigma_z \quad \sigma_{rz} \quad \sigma_\theta]^T$$

$$\{\epsilon\} = [\epsilon_r \quad \epsilon_z \quad \epsilon_{rz} \quad \tau_\theta]^T$$

$$[D] = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu & 0 & \nu \\ \nu & 1-\nu & 0 & 0 \\ 0 & 0 & (1-2\nu)/2 & 0 \\ \nu & \nu & 0 & 1-\nu \end{bmatrix}$$

$$\{P\} = (1+\nu)\alpha\ [1 \quad 1 \quad 0 \quad 1]^T$$

Both the strains and temperatures are required for the solution of stresses in the thermo-mechanical constitutive equation (equation 2.15). Although the equations for conduction heat transfer have been developed in the first part of this chapter, they are repeated along with the development of the thermo-elastic equations to emphasize their co-existence in the domain. Fouriers law, for the plane cases this is

$$\{q\} = -[k]\{g\} \qquad (2.16)$$

where $\{q\} = [q_x \quad q_y]^T$

$$[k] = \begin{bmatrix} k_{11} & k_{12} \\ k_{21} & k_{22} \end{bmatrix}$$

and $[g] = [\partial T/\partial x \quad \partial T/\partial y]^T$

For the steady state equations 2.15 and 2.16, the equations of equilibrium are

$$[d]\,\{\sigma\} = \{0\} \quad \text{- mechanical equilibrium} \qquad (2.17)$$

where $[d] = \begin{bmatrix} \frac{\partial}{\partial x} & 0 & \frac{\partial}{\partial y} \\ 0 & \frac{\partial}{\partial y} & \frac{\partial}{\partial x} \end{bmatrix}$

$$\text{and } \{\delta\}^T\,\{q\} + Q = 0 \quad \text{- thermal equilibrium} \qquad (2.18)$$

Substitution of the constitutive equations, 2.15 and 2.16, into their corresponding equilibrium equations, 2.17 and 2.18 gives the general equations

$$[d][D]\{\epsilon\} - [d][D]\{P\}(T - T_o) = \{0\} \qquad (2.19)$$

$$\text{and} \quad \{\delta\}^T[k]\{g\} + Q = 0 \qquad (2.20)$$

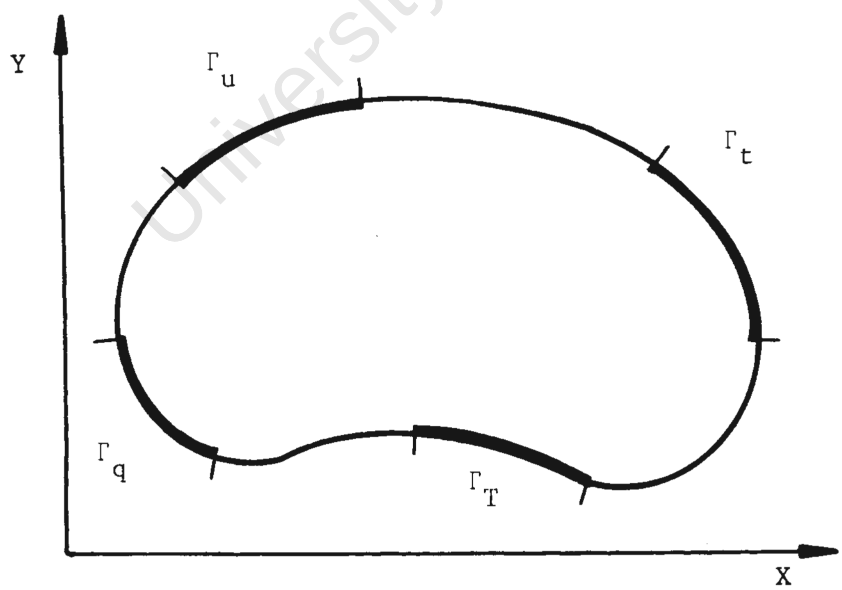


Figure 2.2 Two dimensional domain for thermo-elasticity

Referring to figure 2.2, it must be noted that the mechanical and heat transfer boundary conditions each exist over the complete boundary. The boundary conditions for the complete thermo-mechanical problem are

1. $\{u\} = \{u_0\}$ is a prescribed displacement on Γ_u (2.21a)

2. $\{t\} = \{t_0\}$ on Γ_t (2.21b)

   This is a general traction with x and y components.
   ie $\{t\} = [M]\{\sigma\} = [t_x \ \ t_y]^T$

   where $[M] = \begin{bmatrix} n_x & 0 & n_y \\ 0 & n_y & n_x \end{bmatrix}$

3. $T = T_0$ is a prescribed temperature on Γ_T (2.22a)

4. $\{q\}^T\{n\} = -q$ on Γ_q (2.22b)

   This is a general heat flux in the direction of the outward normal. It may incorporate one or more of the boundary conditions as in equations 2.4a-e.

It can be seen at this stage that equations 2.20 and 2.22 for the heat transfer in the solution region, are independent of equations 2.19 and 2.21, though the reverse is not true. Thus the heat transfer part of the problem can be solved first, and the temperature field solution used in solving equation 2.19 to find mechanical deformations. Note that this includes the possibility of making the material properties for the mechanical part of the analysis temperature dependent.

2.2.3 <u>Finite Element Formulation</u>

The finite element formulation for conduction heat transfer has been developed in section 2.1.4. and the mechanical formulation is now given, assuming known nodal values of temperature.

Galerkin's method is now applied to the mechanical equilibrium equation 2.17.

An arbitrary displacement field $\{\bar{w}\}$, which incorporates displacements in the plane is assumed. Equation 2.17 is multiplied by this field and integrated over the solution domain.

ie $$\int_{\Omega} \{\bar{w}\} [d] \{\sigma\} d\Omega = 0 \qquad (2.23)$$

Using Gauss's theorem to include the boundary conditions, equation 2.27 expands to

$$\int_{\Omega} \{\bar{\varepsilon}\}^T \{\sigma\} dV = \int_{\Gamma_u} \{\bar{w}\}^T \{t\} d\Gamma + \int_{\Gamma_t} \{\bar{w}\}^T \{t_o\} d\Gamma \qquad (2.24)$$

Where $\{\bar{\varepsilon}\}$ is the strain vector corresponding to the displacement field $\{\bar{w}\}$ so that

$$\{\bar{\varepsilon}\} = [d]\{\bar{w}\} \qquad (2.25)$$

The solution domain is divided into M elements of n nodes each, and a general interpolation matrix, [N], consisting of n shape functions, is specified for an element.

$$[N] = [N_1 \; N_2 \; ....N_n] \qquad (2.26a)$$

The corresponding gradient interpolation matrix for strains is

$$[B]_r = \begin{bmatrix} \frac{\partial N_r}{\partial x} & 0 \\ 0 & \frac{\partial N_r}{\partial y} \\ \frac{\partial N_r}{\partial y} & \frac{\partial N_r}{\partial x} \end{bmatrix} \quad \text{for } r = 1,2 \; ....n \qquad (2.26b)$$

Using the interpolation functions, the displacement in an element can be expressed by

$$\{w\}^{(e)} = \begin{Bmatrix} u(x,y) \\ v(x,y) \end{Bmatrix}^{(e)} = \begin{Bmatrix} [N]\{u\} \\ [N]\{v\} \end{Bmatrix}^{(e)} = [N]\{\bar{a}\}^{(e)} \qquad (2.27)$$

where $\{\bar{a}\}$ is the general nodal displacement vector corresponding to the displacement vectors $\{u\}$ and $\{v\}$ in the x and y directions.

Similarly, the strain field $\{\epsilon\}$ in equation 2.15 is approximated by

$$\{\epsilon\} = [d]\ \{w\}^{(e)} \qquad (2.28)$$

where the nodal displacements $\{w\}^{(e)}$ are

$$\{w\}^{(e)} = [N]\ \{a\}^{(e)} \qquad (2.29)$$

Equations 2.27 and 2.29 show the principal difference between the finite element formulation for the mechanical case now considered and that for the heat transfer case as presented in section 2.14. In the heat transfer case the unknown temperature was a scalar, but in this case the field variable, displacement, is a vector.

The strain vector in equation 2.25 can be written in terms of the interpolation functions as

$$\{\bar{\epsilon}\}^{(e)} = [d][N]\{\bar{w}\}^{(e)} = [B]\{\bar{a}\}^{(e)} \qquad (2.30)$$

The expressions for $\{\epsilon\}$ and $\{\bar{\epsilon}\}$ are substituted into equations 2.15 and 2.24 respectively to give

$$\{\sigma\} = [D][B]\{a\}^{(e)} - [D]\{P\}(T - T_o) \qquad (2.31)$$

and
$$\int_{\Omega} [B]^T\{\bar{a}\}^{(e)T}\{\sigma\}d\Omega = \int_{\Gamma_u} \{\bar{a}\}^{(e)T}[N]\{t\}d\Gamma + \int_{\Gamma_t} \{\bar{a}\}^{(e)T}[N]\{t_o\}d\Gamma \qquad (2.32)$$

In equation 2.32 $\{\bar{a}\}^{(e)}$ is common to all terms and hence arbitrary. Removing $\{\bar{a}\}^{(e)}$ and substituting equation 2.31 into equation 2.32 gives

$$[K]\{a\} - \{L\} = \{F_u\} + \{F_t\} \tag{2.33}$$

where $[K] = \int_{\Omega} [B]^T[D][B]d\Omega$ - Mechanical stiffness matrix

$\{L\} = \int_{\Omega} [D][B]\{P\}(T - T_o)d\Omega$ - Thermal strain equivalent load vector

$\{F_u\} = \int_{\Gamma_u} [N]\{t\}d\Gamma$ - Constraint boundary reactions

$\{F_t\} = \int_{\Gamma_t} [N]\{t_o\}d\Gamma$ - Mechanical loads

Apart from the thermal contribution, {L}, equation 2.33 takes the form of the purely nechanical temperature independent problem described in detail by Heubner[4], Bathe[21] and Owen and Hinton[22].

The uncoupled nature of the problem developed here means that the temperature field is determined for its steady state final condition before any thermal strain loads {L} are applied to the mechanical system.

If the thermal stresses induced by this final temperature field are sufficiently large to produce a nonlinear mechanical response then the thermal loads must be applied incrementally. This approach of dividing the thermal loads due to a final temperature field into increments which are then applied sequentially is demonstrated by

Grill[23].

Isotropic expansion coefficients have been assumed in this formulation, but Wu[24] shows how this can be modified to accommodate for a completely anisotropic material.

In summary, an uncoupled finite element formulation for steady state thermo-mechanical stress analysis has been derived in this chapter. Thus, the temperature distribution for a solution domain can be determined completely before it is applied to the same domain with the same discretization in order to determine the stress field.

CHAPTER THREE

NUMERICAL IMPLEMENTATION

3.1 INTRODUCTION

Developments in finite element analysis have grown with the availability of mass computational facilities. Beyond the classroom the method's ability is only an asset if it is installed on a computer of reasonable size. For this thesis the formulations of the previous chapter were implemented into the existing finite element stress analysis code, NOSTRUM(1).

The intention was to extend the ability of NOSTRUM to include heat transfer analysis and the possibility of temperature changes in the mechanical stress analysis procedures where previously all analysis was considered independent of temperature. Two dimensional isoparametric finite continuum elements were used for the extensions.

This chapter deals with the implementation of the heat transfer analysis mode, and the consequent thermo-mechanical strains. This is done in general terms which could be applied to many stress codes. The actual implementation done in NOSTRUM for this thesis runs to approximately 3100 lines, of which 600 are incorporated in existing routines and the balance of 2500 form newly developed routines.

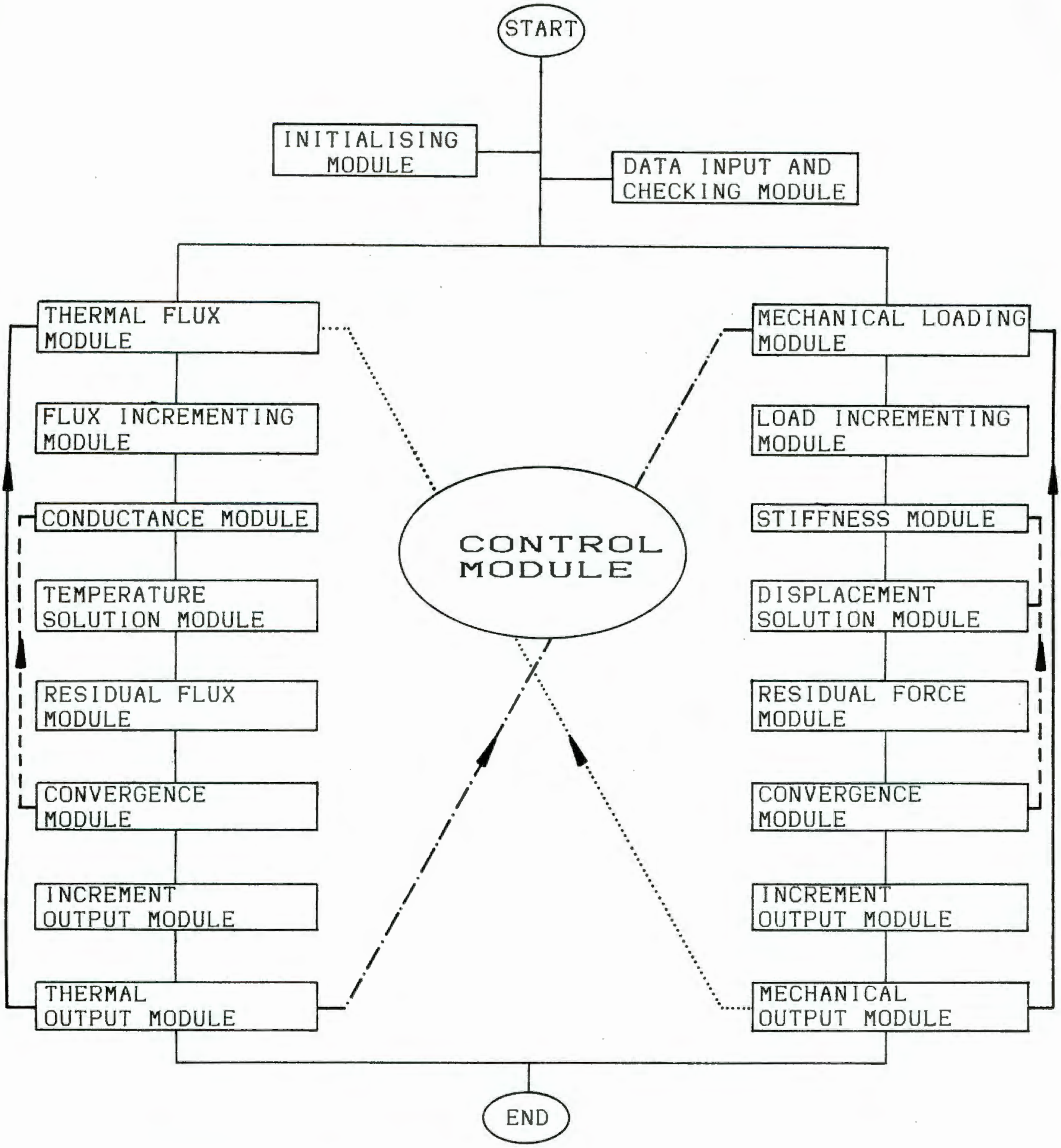
A synopsis of the programming done is given in Appendix A, and the reader is referred to the Applied Mechanics Research Unit at the University of Cape Town for actual listings.

3.2 PROGRAM STRUCTURE

NOSTRUM is written in modular format so that separate subroutines perform distinct tasks at the various levels of the organization and computation in the program. It was decided to utilize as many of the existing routines as possible, and therefore to integrate the heat transfer solution modules into the present structure.

The alternative to this approach was to construct a "separate" heat transfer program to solve for temperatures, which would then be passed across to the input of the stress analysis program. This would eliminate the need to develop a finite element code as one of the many published codes could be used, and then only the management of the combined system need be tackled. This has two distinct disadvantages. One is that a separate data deck would be required for each program, which apart from the inconvenience to the user, also detracts from the concept of introducing a further dimension of temperature, (extra degree of freedom) to each node of the model. The second is that any extensions to the combined programs for the fully coupled thermo-mechanical problem would introduce added complications to control procedures.

The version of NOSTRUM incorporating the work of this thesis will be referred to as NOSTRUM/THERMAL. The program structure is shown schematically in figure 3.1. This shows the use of common control, initializing and input modules, and the symmetry of the mechanical and thermal nonlinear analysis paths. Uncoupled thermo-mechanical analysis is performed by sequential thermal and then mechanical analyses. A possible path for extension to the coupled problem is indicated. This is, however, a simplification of the problem as it also requires its own incremental and iteration loops which if drawn in would make the figure confusing.



——— Time Step Loops
- - - - - Iteration Loops
—·—·—· Uncoupled Thermo-Mechanical Path
.... possible path for coupled analysis

Figure 3.1 Program modules for nonlinear thermo-mechanical code, NOSTRUM/THERMAL

From figure 3.1 it can be seen that the mechanical analysis path is only affected by the thermal analysis in its loading module. This is the only module in the mechanical path which is specifically discussed in this chapter.

Most of the nonlinear mechanical routines were developed by Owen and Hinton[22] and an overview of NOSTRUM is given by Duffett *et al*[1].

At this stage it is assumed that the reader has a knowledge of the basics of finite element programming and isoparametric element terminology. Specific instructions on programming methods is given by Hinton and Owen[25], but this is also dealt with in the finite element texts[2,3,4,21] already mentioned.

The common modules of initializing, input and checking required adjustment for the inclusion of the heat transfer mode. These changes, where relevant to the thermo-mechanical concept, are discussed. Although no coded programs are presented here, the computer language and style used do have an influence on the method of computation and some aspects are now mentioned.

The programming was done in FORTRAN. For readability variable names were constructed so as to be either abbreviations or have onomatopoeic resemblance to the standard terminology. Many of the "housework" operations necessary in mechanical finite element analysis, such as global degrees of freedom numbering, are eliminated for heat transfer analysis because temperature is the only degree of freedom at each node.

Since isoparametric elements are used, element matrices are computed by numerical (as opposed to explicit) integration. The Gauss Quadrature technique used is standard in practice and has the advantage that reduced integration can be used to overcome problems such as "locking".

3.3 MODEL INPUT

A common finite element model is used for both the heat transfer and mechanical analyses. Hence the common input acceptance routine must "gather" the model data for the following analysis type possibilities:

1) Purely mechanical analysis
2) Purely heat transfer analysis
3) Thermo-mechanical analysis.

It was seen in figure 3.1 that the addition of the thermal aspect to a mechanical code requires additional control from the control module in order to guide the solution process through one of the above three possibilities. Further data specific to heat transfer analysis is also required.

The input data can be sub-divided into four main classifications:

1) The control data which is used for; selection in the type of data required in the other three classifications; setting up of solution strategy and procedures; and determining output selections.
2) The data required to define the geometry of the model and its boundary conditions.
3) The properties and material laws of the models constituent materials.
4) The heating and mechanical loading to which the model is subjected.

Figure 3.2 shows the route of data input to NOSTRUM/ THERMAL.

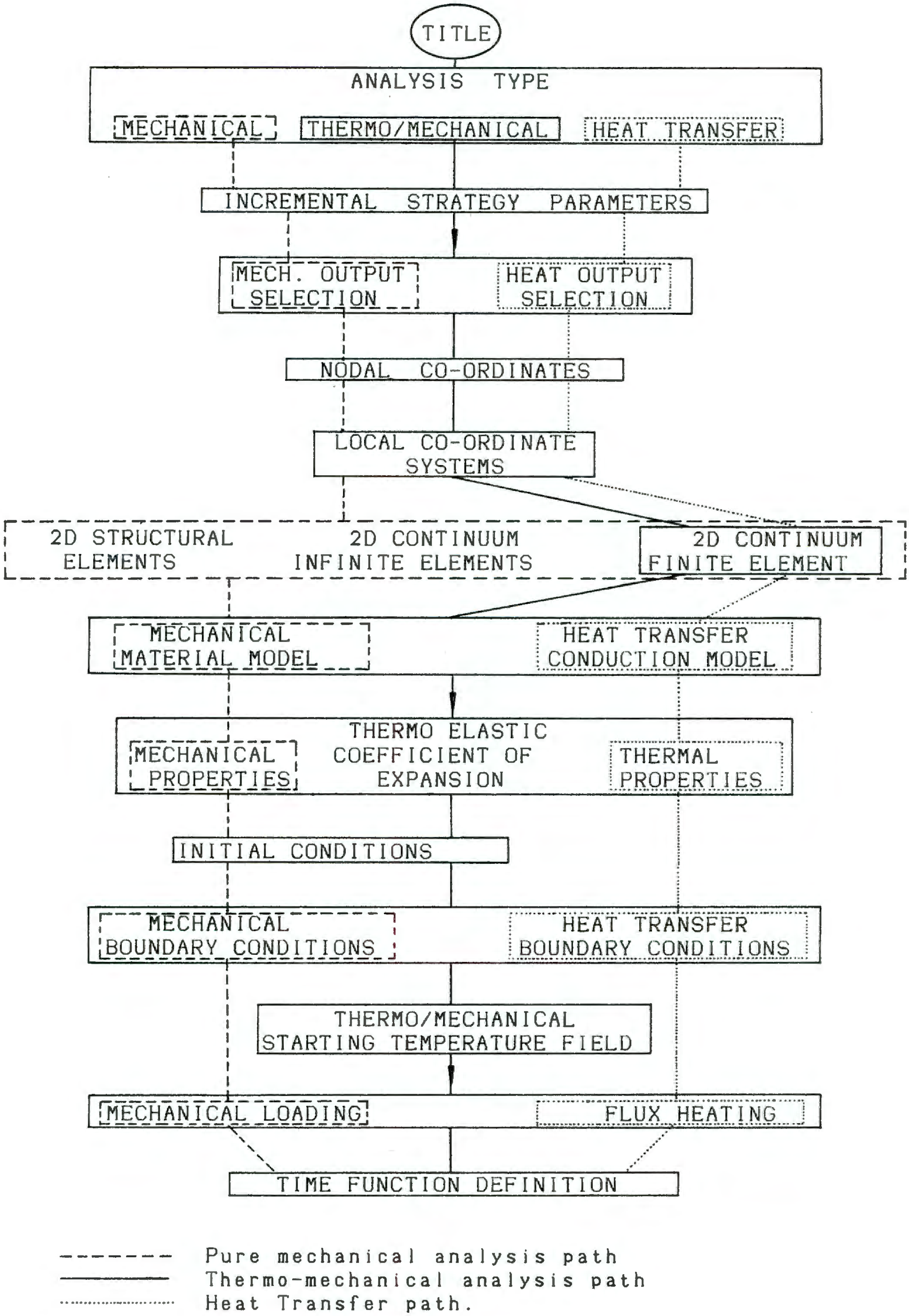


Figure 3.2 Schematic chart of data input for NOSTRUM/THERMAL

At most stages of the input the heat transfer data is merely a parallel to the corresponding mechanical data and the thermo-mechanical a combination of the two. Notable differences are the absence of initial conditions, and the use of only two dimensional finite elements in heat transfer, and that the specification of a starting temperature field for thermo-mechanical analysis is possible. The latter has three options.

1) A known temperature field can be specified and the corresponding thermal strains and stresses then computed.
2) A starting temperature field can be specified (at which no thermal strains are present), and this, subtracted from the temperature field obtained by heat transfer analysis, leads to a strain field caused by the change.
3) An uniform temperature field can be specified and the strains computed from the difference between this field and that determined in a heat transfer analysis.

The input of data for nonlinear materials is also different from the present NOSTRUM type format. For a material which has a purely linear relationship with temperature of the type: Property = a + bT, the values of a and b are simply entered. However, in many realistic cases an empirical curve will represent the variation of the property. For these cases the method used by Thornton (15) and Hibbitt et al (26) has been implemented. Here, the curve is piecewise approximated by as many straight lines as necessary. The input required is a series of sets of values of property and corresponding temperature. The program interpolates linearly to obtain the specific value at any temperature. Should the value of the temperature lie outside the specified range, then the nearest specified value is assumed and a suitable warning message given.

Nonlinear thermal conductivity and material internal heat generation are accounted for in this manner in NOSTRUM/THERMAL.

Details of the input required may be found in the user manual [27]

3.4 HEAT TRANSFER ELEMENT EQUATIONS

This section describes the computation sequence used to obtain the flux vectors and conductance matrices of the elements. The description is general and does not use the particular notation of variable and subroutine names used in NOSTRUM/THERMAL. A flow chart for the Heat Transfer section of NOSTRUM/THERMAL giving actual subroutine names and purpose is tabled in appendix A. This also shows the breakdown of tasks to be performed by lower order subroutines.

3.4.1 Conductance Matrix

The conductance matrix corresponds to the stiffness matrix in stress analysis. For the general nonlinear heat transfer case given by equation 2.11 it has components due to conduction, convection and radiation. For the purposes of this thesis only the components due to conductivity are considered.

The expression for the conductivity component of the conductance matrix $[C_c]$ is adjusted for isoparametric representation by introducing the Jacobian and integrating in the natural co-ordinate system to give

$$[C_c] = \int_{-1}^{+1} \int_{-1}^{+1} t[B(\xi,\eta)]^T [k(T)][B(\xi,\eta) \; |J(\xi,\eta)] \, d\xi d\eta \qquad (3.1)$$

where : t is the element thickness in plane stress (It is neglected for plane strain and axisymetric cases)

: $[B(\xi,\eta)]$ is the temperature gradient matrix in natural co-ordinates ξ and η.

: [k(T)] is the conductivity matrix. Note that for nonlinear conductivity, this matrix is evaluated at the temperature (T) of the position (ξ,η) in the element. For the first iteration in a nonlinear problem this will be evaluated at the conductivity corresponding to zero temperature.
$|J(\xi,\eta)|$ is the determinant of the Jacobian matrix.

The components of $[C_e]$ are evaluated numerically. Letting the integrand in equation (3.1) be denoted as [H], and introducing Gaussian Quadrature for a quadrilateral element with NG x NG sampling points leads to

$$[C_e] = \sum_{i=1}^{NG} \sum_{j=1}^{NG} W_i W_j \, [H(\xi_i, \eta_{j\,i})] \qquad (3.2)$$

where W_i and W_j are weighting factors and $[C_e]$ is evaluated at sampling positions ($\xi_i, \eta_{j\,i}$). The main steps of the computer implementation of equation 3.2 are shown in figure 3.3.

Call routine to set up sampling point positions and weighting factors for numerical integration

Enter loop over all elements

Retrieve element geometry and temperatures from the previous iteration and material properties for the current element

Zero the conductance array

Enter loops covering all integration points

Determine the sampling position of the current integration point (ξ,η).

Call routine to supply shape functions and their derivatives at the sampling point.

Pass sampling point position, shape functions and derivatives to subroutine which calculates the Jacobian matrix [J], its inverse $[J]^{-1}$, its determinant |J| and the global co-ordinates (x,y) of the sampling point.

Calculate the temperature at the sampling point

Call the routine to evaluate the conductivity matrix [k] for the temperature at the sampling point.

Call the temperature gradient matrix routine to evaluate [B] at the sampling point.

Call the routine to multiply the conductivity and temperature gradient matrices [k][B].

Evaluate $[B]^T[k][B]\times|J|$ x integration weights and assemble them into the element conductance array.

End integration loop

Write conductance matrix to file for use in solution routine.

End Element Loop

Figure 3.3 Evaluation of the element conductance matrix for numerically integrated isoparametric elements.

3.4.2. Flux Vector

As with loading in the finite element analysis of structures by the displacement method, the only possible method of including heating in heat transfer by finite elements, other than by prescribing boundary temperatures, is by the application of concentrated fluxes at nodal points. Consequently the types of heating derived in chapter 2 must be reduced to equivalent nodal fluxes before the solution can be performed.

For isoparametric elements the calculation of these fluxes cannot be performed manually since area or volume integrations over randomly shaped regions are usually required. Therefore these equivalent fluxes cannot be included at the data input stage.

In this section the computational procedures for internal heat generation and edge flux heating are shown.

Convection (which can be approximated by specified edge heating) and radiation exchange have been omitted. Point source heating, while included in NOSTRUM/THERMAL, is not discussed as it is accounted for by simply adding the specified values to the relevant node in the flux vector.

Internal Heat Generation

The internal heat generation component of the flux vector specified in equation 2.11 is rewritten for isoparametric representation. Numerical integration is introduced to give for the flux at node r,

$$R_{e\,r} = \sum_{i=1}^{NG} \sum_{j=1}^{NG} Q(T)\, N_r(\xi,\eta)\, W_i\, W_j\, |J(\xi,\eta)| \qquad (3.3)$$

where N_r is the shape function corresponding to node r and Q is the value of internal heat generation, which will normally be a material property and may be a function of temperature. As with the dependence of conductivity on temperature, the variation of Q with temperature has no effect on the calculation of the initial flux vector because zero temperatures are assumed at the start of an analysis. Any variation of Q with temperature is used in updating the flux vector for the determination of the residual or out of balance fluxes.

The main steps of the computer implementation of equation 3.3 are shown in figure 3.4.

Call routine to set up sampling point positions and weighting factors for numerical integration

Enter loop over all elements

Retrieve element geometry and temperatures from the previous iteration, and relevant material properties for the current element.

Enter loops covering all integration points

Determine the sampling position of the current integration point (ξ,η)

Call routine to supply shape functions and their derivatives at the sampling point.

Call routine to calculate the Jacobian matrix [J], its inverse $[J]^{-1}$, its determinant |J| and the co-ordinates (x,y) of the sampling point.

Calculate the temperature at the sampling point.

Call routine to evaluate Q at the sampling point temperature.

Evaluate Q(T) N_r x |J| x integration weights and assemble into element flux vectors.

End integration loop

End Element loop.

Figure 3.4 Evaluation of the components of the element flux vector due to internal heat generation for isoparametric elements

<u>Edge Flux Heating</u>

The prime difference between internal heat generation and edge flux heating is that the latter is integrated over the boundary of the element and not the area or volume. This means that only one of the local directions (ξ,η) need be considered. ξ is used here.

Suppose that ℓ nodal values of flux are given at ℓ nodal points along an element edge. Then the intensity at any point on that edge is found by using the shape functions corresponding to such an element of interpolation degree ℓ so that on a boundary with specified flux

$$q = \sum_{r=1}^{\ell} N_r \; q_r \qquad (3.4)$$

Consider this flux to act on an edge of incremental length $d\Gamma$. The edge, $d\Gamma$, is inclined at an angle β to the x axis. (see figure 3.5)

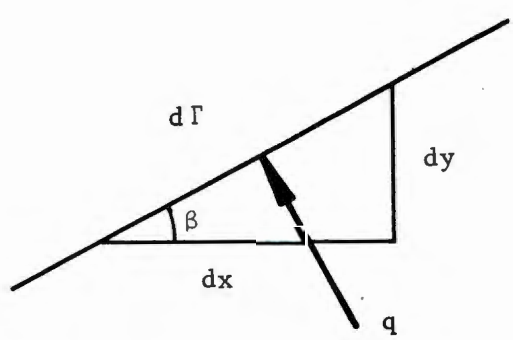


Figure 3.5 Inclined edge of isoparametric element

The incremental flux corresponding to $d\Gamma$ is

$$dR_q = q_s \, d\Gamma \cos\beta + q_s \, d\Gamma \sin\beta$$
$$= q_s (dx + dy) \qquad (3.5)$$

Since an isoparametric representation is used, integration is performed along this edge in terms of the curvilinear variable ξ. Thus

$$dx = (\partial x/\partial \xi)d\xi \text{ and } dy = (\partial y/\partial \xi)d\xi \qquad (3.6)$$

Substituting equations 3.6 into equation 3.5 gives,

$$dR_q = q_s (\partial x/\partial \xi - \partial y/\partial \xi)d\xi, \qquad (3.7)$$

and the corresponding equivalent nodal fluxes are

$$R_{q\,r} = \int_\Gamma N_r(\xi,\eta) q_s (\partial x/\partial \xi - \partial y/\partial \xi)d\xi \qquad (3.8)$$

Applying numerical integration to equation 3.8 gives

$$R_{q\,r} = \sum_{i=1}^{NG} q_s \; N_r(\xi,\eta)(\partial x/\partial \xi - \partial y/\partial \xi)W_i \qquad (3.9)$$

As with internal heat generation, specified edge flux could be made temperature dependent. However, in many engineering applications it will be a constant known input of energy and has been left as such in NOSTRUM/THERMAL.

The main steps of the computer implementation of equation 3.9 are shown in figure 3.6

Enter loop for each specified edge flux.

Locate element being heated by association of the nodes corresponding to the flux.

Call routine which calculates consistent nodal flux values on the element.

Call routine to set up sampling point positions and weighting factors for numerical integration.

Enter loop covering the integration points.

Retrieve element geometry and relevant material properties for the affected element.

Determine the sampling position of the current integration point (ξ).

Call routine to supply shape functions and their derivatives at the sampling point.

Enter loop to calculate the value of q at the sampling point from equation 3.4.

Evaluate the derivatives ($\partial x/\partial \xi$ and $\partial y/\partial \xi$) at the sampling point.

End Loop.

Evaluate $q_{\bullet}\, N_r(\partial x/\partial \xi - \partial y/\partial \xi)$ (Let this equal A^*)

Locate which side of the element is being heated.

Evaluate A^* x weighting factor and assemble into the correct location of the flux vector.

End integration loop

End edge flux loop

Figure 3.6 Evaluation of the components of the element flux vector due to edge flux heating

3.5 SOLUTION OF NONLINEAR HEAT TRANSFER EQUATIONS

Nonlinear heat transfer problems arise when material properties are dependent on temperature.

Direct solution of the system of equations

$$[C^{(T)}]\{T\} = \{R\} \qquad (3.10)$$

which is representative of equation 2.13 is generally impossible and an iterative scheme must be used.

A direct iterative scheme based on the Newton-Raphson method has been used in NOSTRUM/THERMAL. In this section the direct iterative scheme is presented. It is followed by the Newton-Raphson Method and its use in the form of a direct iterative scheme.

In the direct iterative method successive solutions are performed, in each of which the previous solution for the temperature field is used to predict the current values of the conductance matrix, [C], and the flux vector {R}. Rewriting equation (3.10) as

$$\{T\} = [C(T)]^{-1}\{R(T)\} \qquad (3.11)$$

the iterative process yields the $(p+1)^{th}$ approximation to be

$$\{T\}^{p+1} = [C(T^{p})]^{-1} \quad \{R(T^{p})\} \qquad (3.12)$$

If the process is convergent, then in the limit as p tends to infinity, $\{T\}^{p}$ tends to the true solution.

The algorithm for the Newton-Raphson Method is

$$[J]^{p}\{\Delta T\}^{p+1} = -\{S\}^{p} \qquad (3.13)$$

and $\{T\}^{p+1} = \{T\}^{p} + \{\Delta T\}^{p+1}$ (3.14)

where $\{S\}^{p}$ is the unbalanced or residual flux vector and $[J]$ is the Jacobian. The flux vector $\{S\}^{p}$ is evaluated from

$$\{S\}^{p} = [C(T^{p})]\{T^{p}\} - \{R(T^{p})\} \qquad (3.15)$$

The r^{th} component of $\{S\}$ for an element with n nodes is given by

$$S_r = \sum_{j=1}^{n} C_{rj}\,T_j - R_r \qquad (3.16)$$

which permits computation of the Jacobian by the definition $J_{rj} = \partial S_r/\partial T_j$. Since C_{rj} is a function of T_j, the term within the summation in equation 3.16 can be differentiated as a product to produce the result

$$[J] = [C] + [\Delta C] - [\Delta R] \qquad (3.17)$$

where $\Delta C_{rj} = \sum_{m=1}^{n} (\partial C_{rm}/\partial T_j)\,T_m$

and $\Delta R_{rj} = \partial R_r/\partial T_j$

The Jacobian matrix is therefore composed of three parts. The $[\Delta C]$ and $[\Delta R]$ parts are non symmetric and the iterative solution consequently requires a non symmetric equation solver .

If $[\Delta C]$ and $[\Delta R]$ are ignored equation (3.13) becomes

$$[C(T^p)]\ \{\Delta T\}^{p+1} = -\{S\}^p \qquad (3.18)$$

Substituting equation 3.14 and 3.15 into 3.18 and rearranging leads to

$$\{T\}^{p+1} = [C(T^p)]^{-1}\{R(T^p)\} \qquad (3.19)$$

which is exactly the same as equation 3.12, the equation for the direct iterative scheme.

The solution method used in NOSTRUM/THERMAL is essentially this direct iterative scheme of equation 3.19 but it has been implemented in the Newton-Raphson format. The solution therefore proceeds by calculation of temperature increments, as in equation 3.13, due to residual fluxes caused by the nonlinearities.

This is intended to lead to conversion of the program to the full Newton-Raphson scheme by the inclusion of the $[\Delta C]$ and $[\Delta R]$ terms in the Jacobian matrix, and development of a non symmetric equation solver for the nodal temperatures.

The computational procedure for the iterative method used in NOSTRUM/THERMAL is shown in figure 3.7

Call routine to evaluate nodal fluxes due to specified heating : $\{R_q\}$

Enter iteration loop.

Call routine to evaluate conductance matrix at temperature field : $[C(T^p)]$

1st iteration - Solve for temperature field due to heating ie $\{T\}^{p+1} = [C(T^p)]^{-1} \{R_q\}$

Subsequent iterations - Solve for temperature increments $\{\Delta T\}^{p+1}$ due to the residual fluxes $\{S\}^p$

Update the temperature field: $\{T\}^{p+1} = \{T\}^p + \{\Delta T\}^{p+1}$

Update the reaction fluxes: $\{RF\}^{p+1} = \{RF\}^p + \{\Delta RF\}^{p+1}$

Include reaction fluxes in the flux vector:

$$\{R\}^{p+1} = \{R\}^p + \{\Delta RF\}^{p+1}$$

Evaluate the new nodal fluxes due to their temperature dependence ie $\{R_q(T^{p+1})\}$. Include any change from $\{R_q\}$ in the flux vector ie $\{R\}^{p+1} = \{R\}^{p+1} + (\{R_q(T^{p+1})\} - \{R_q\})$

Evaluate the internal fluxes due to the new field $[C(T^{p+1})] \{T\}^{p+1}$

Evaluate the residual fluxes which are the differences between the updated flux vector and the internal fluxes:

$$\{S\}^{p+1} = \{R\}^{p+1} - [C(T^{p+1})] \{T\}^{p+1}$$

Check for convergence by evaluating norm of residual fluxes and comparing with tolerance specified by user.

End iteration loop.

Figure 3.7 Computation sequence for iteration method

3.6 THERMO MECHANICAL PROCEDURES

The theory behind uncoupled thermo-mechanical analysis has been developed in Chapter 2. As has been mentioned there, the only effect that this has on a temperature independent finite element stress analysis procedure is the imposition of thermal strain loads.

These loads are calculated from the strains due to the temperature changes over the solution region and are added to the load vector in the same way that the loads due to initial mechanical strains are added.

For implementation in NOSTRUM/THERMAL, the selection in the control data of a thermo-mechanical type of analysis ensures that the routines which are used in applying initial strain loads are called. This happens whether a specified temperature change field has been input or whether a field has been determined by heat transfer analysis.

A flow chart of the computational scheme used in assembling the thermal strain loads is shown in figure 3.8

Nonlinear deformation occurring due to the thermal strain loads is already accounted for in NOSTRUM by the incremental loading procedure which is used in nonlinear stress analysis. This procedure is documented by Owen and Hinton [22] and in the NOSTRUM Theoretical Manual[28]

Thermo-mechanical analysis with NOSTRUM/THERMAL may therefore utilize the various constitutive plasticity laws available. At this stage however, no accommodation has been made for temperature dependence of any of the material properties used in these laws.

Call routine to set up sampling point positions and weighting factors for numerical integration.

Loop over all elements

Retrieve element geometry and material properties for the current element.

Determine the temperature field to be applied to the model.

Call routine which sets up the elasticity matrix,[D]

Enter loops covering all integration points.

Locate the sampling position for the current integration point (ξ,η)

Call routine to supply shape functions and their derivatives at the sampling point.

Call routine which calculates the Jacobian matrix [J], its inverse $[J]^{-1}$, its determinant |J| and the global co-ordinates (x,y) of the sampling point.

Evaluate the temperature at the current sampling point.

Evaluate the initial thermal strains $\{\epsilon_T\} = \{P\}T$

Call the strain matrix routine which returns [B]

Call routine to multiply the elasticity and strain matrices [D] [B]

Assemble the total imposed strain vector (ϵ = initial strains + thermal strains)

Calculate [D] [B] $\{\epsilon\}$ x |J| x integration weights and assemble into imposed strain load increment.

End integration loops

End element loop

Figure 3.8 Evaluation of imposed thermal strain loads for numerically integrated isoparametric elements.

CHAPTER FOUR

ILLUSTRATIVE EXAMPLES

Examples demonstrating the theory and numerical implementation are shown in this chapter. They are compared with exact solutions from the literature.

4.1 NONLINEAR HEAT CONDUCTION IN A SQUARE PLATE

A square plate was subjected to a sinusoidal temperature distribution along one edge, while the others were kept at zero temperature. The thermal conductivity was assumed to vary linearly with temperature according to $k = k_o(1 + 0.5T)$.

The finite element model used is shown in figure 4.1 where for generality the plate has unit dimensions and $k_o = 1$

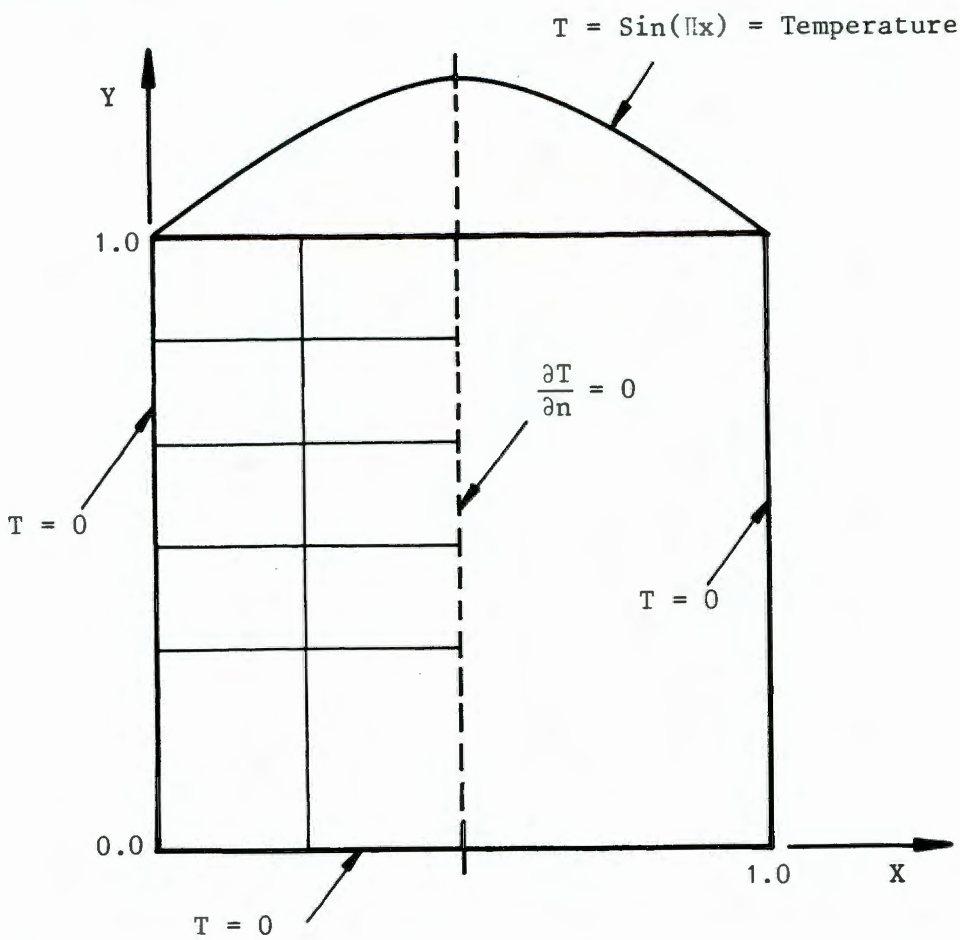


Figure 4.1 Heat conduction through a square plate indicating boundary conditions and the finite element mesh used.

For this problem, results of a variational method solution by Hays and Curd[11] were available. Figure 4.2 shows the finite element results where three iterations were required to achieve a one per cent convergence tolerance. As can be seen, the finite element temperatures are in excellent agreement with the variation results.

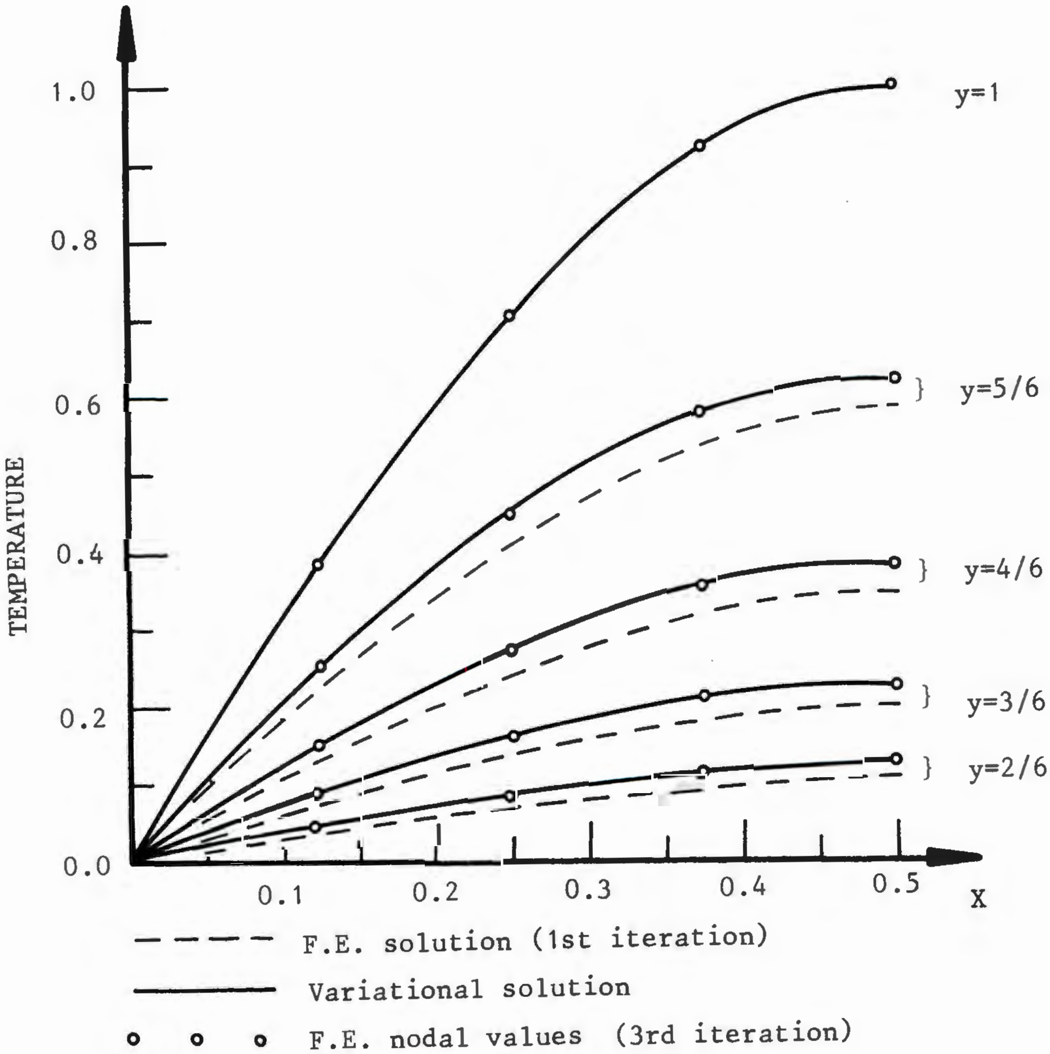


Figure 4.2 Temperature distribution across various sections of square plate

4.2 HEAT TRANSFER AND STRESS ANALYSIS OF A COMPOSITE CYLINDER

The temperature gradient through the wall of a composite cylinder is computed in this example.

The cylinder is composed of three different materials, each with temperature dependent conductivities. The conductivity/temperature relationships for the materials are

$$k_1 = 7\times10^{-2} - 5\times10^{-5}T + 3\times10^{-8}T^2 - 5\times10^{-12}T^3 + 3\times10^{-16}T^4$$

$$k_2 = 2\times10^{-2} + 5\times10^{-5}T - 10^{-8}T^2$$

$$k_3 = 10^{-1} + 4\times10^{-4}T \text{ (W/cm°C)}$$

The interface contact resistances are assumed negligible, and the tube operates between a uniform internal temperature of 2000°C and an external temperature of 0°C. The problem is modelled using 10 axisymetric elements as shown in figure 4.3.

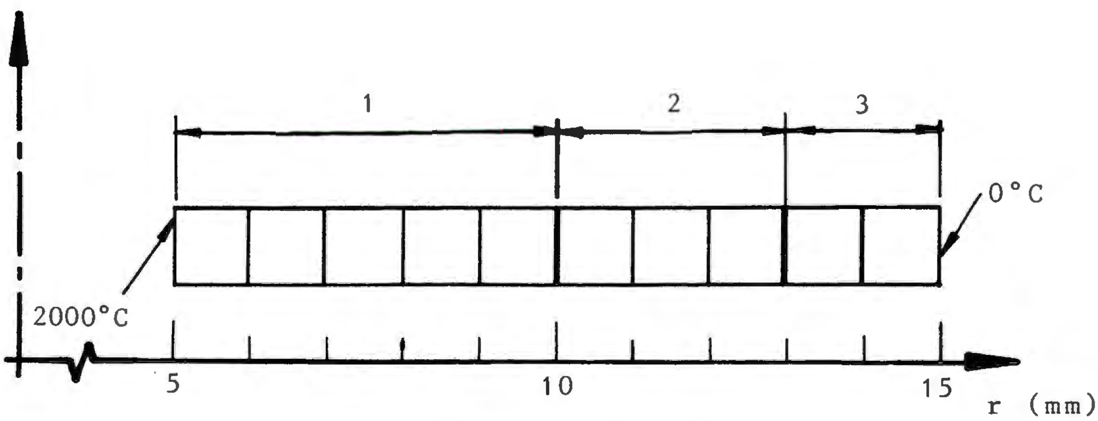


Figure 4.3 Finite element model for composite cylinder

The solution converged to a tolerance of 1% in four iterations and the results are plotted with the exact analytical solution given by Donea[29] in figure 4.4.

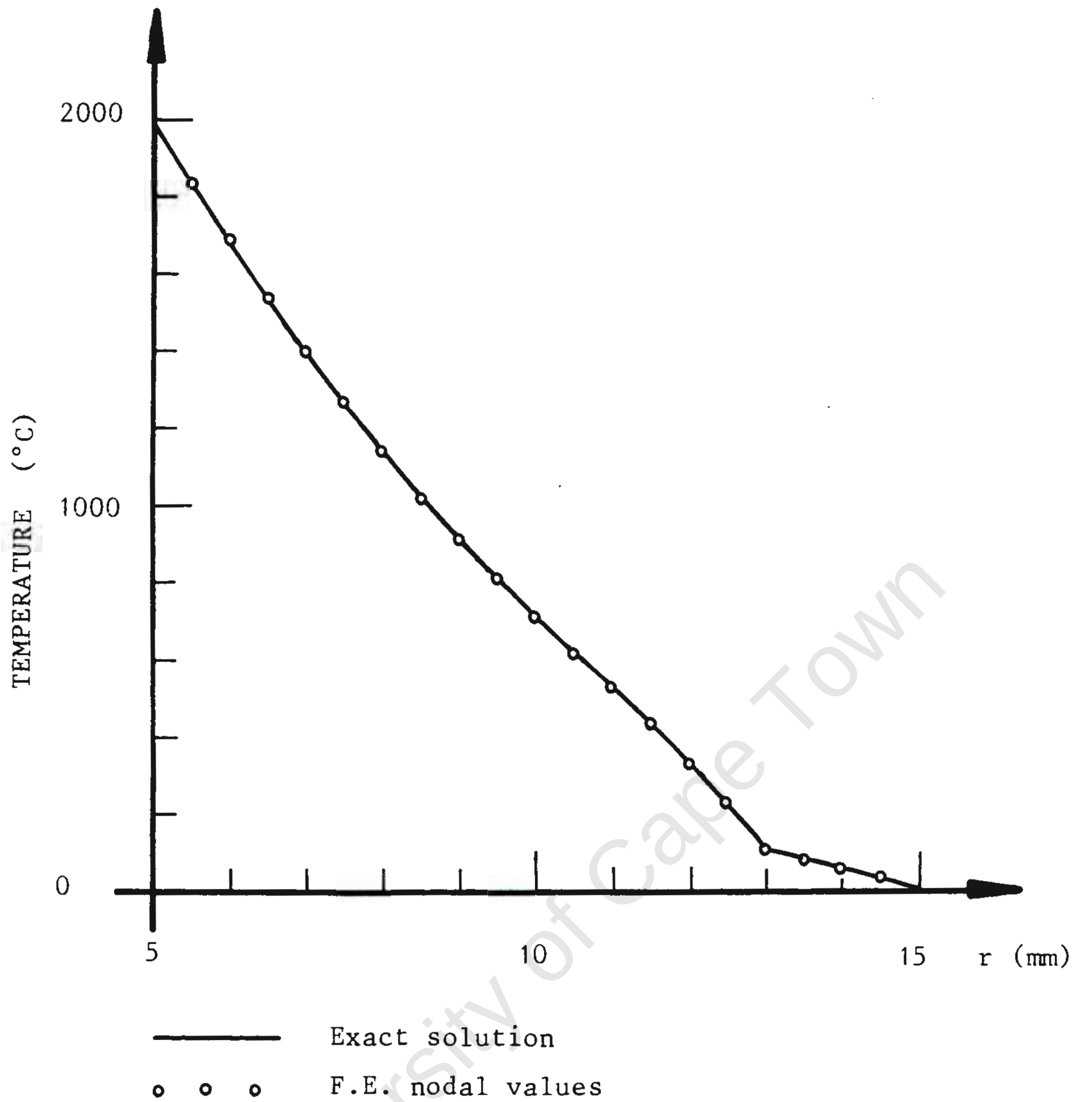


Figure 4.4 Radial temperature profile in the composite cylinder

The radial, hoop and axial stresses for the cylinder are plotted in figure 4.5 and compared with analytical solutions presented by Boresi[30].

For the purpose of the example the following material properties were assumed:

	E (MPa)	ν	α ($°C^{-1}$)
Material 1	1.2	0.36	1.2×10^{-3}
Material 2	1.0	0.3	1.0×10^{-3}
Material 3	0.8	0.24	0.8×10^{-3}

In addition to the thermal loads, a pressure of 1 MPa was applied on the inside wall while the outer wall was left unloaded.

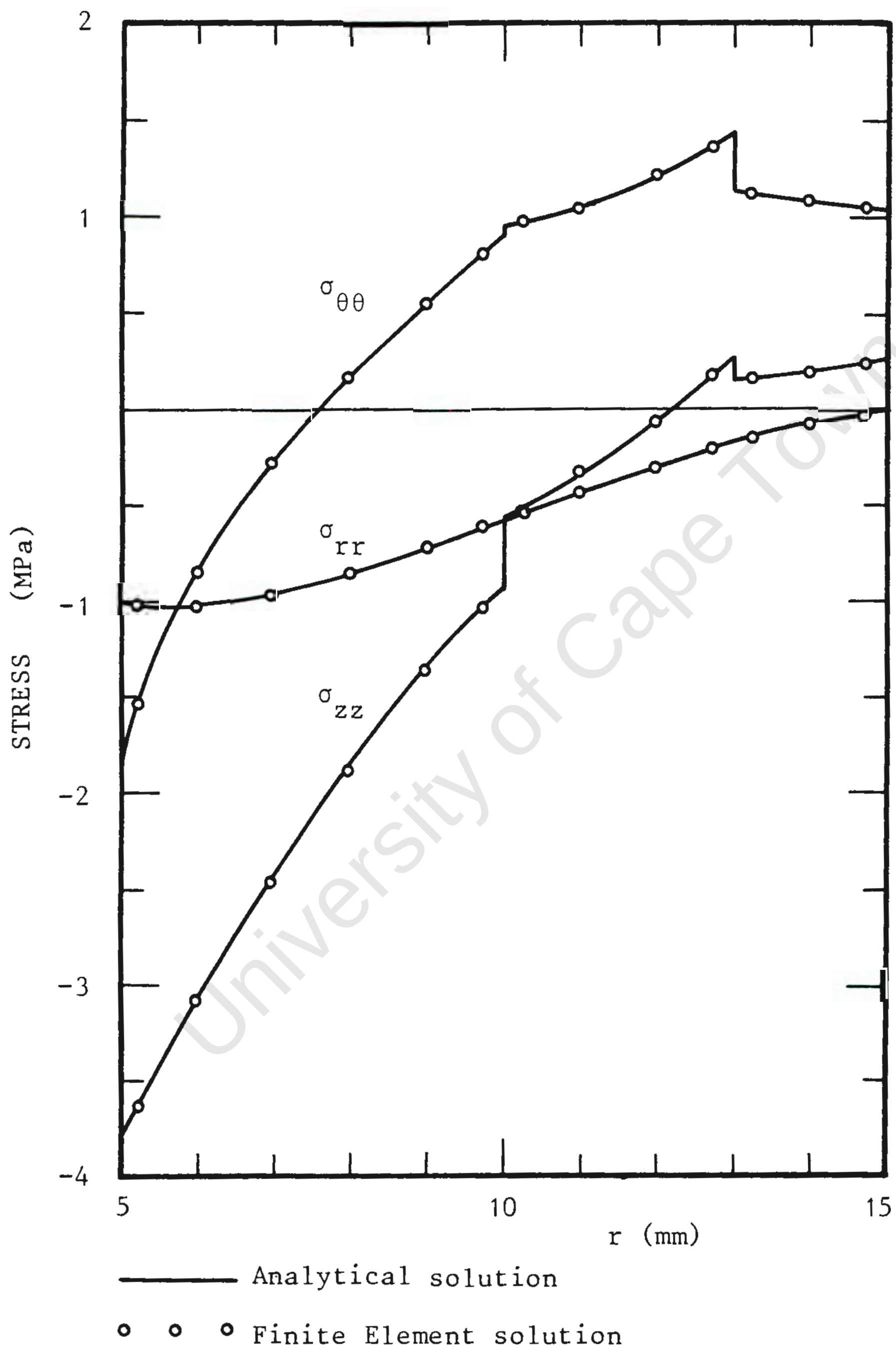


Figure 4.5 Stress distribution in composite cylinder with thermal straining and internal pressure.

Again, the numerical solutions are in excellent agreement with the analytical solutions.

4.3 DEFORMATION OF HEAT GENERATING CYLINDERS

This example demonstrates the accuracy of the program in predicting thermal stresses and displacements in finite heat generating circular cylinders. This is one of the most common thermal stress computations made in the nuclear industry where fuel pellets deform under their own heat generation. Even though these pellets in most cases have an effectively radial temperature distribution, as they are stacked one on top of another, the axial mid plane is the only region of purely radial deformation.

The model and terminology used in this example are shown in figure 4.6. The radius ratio is defined as $\rho = r/b$.

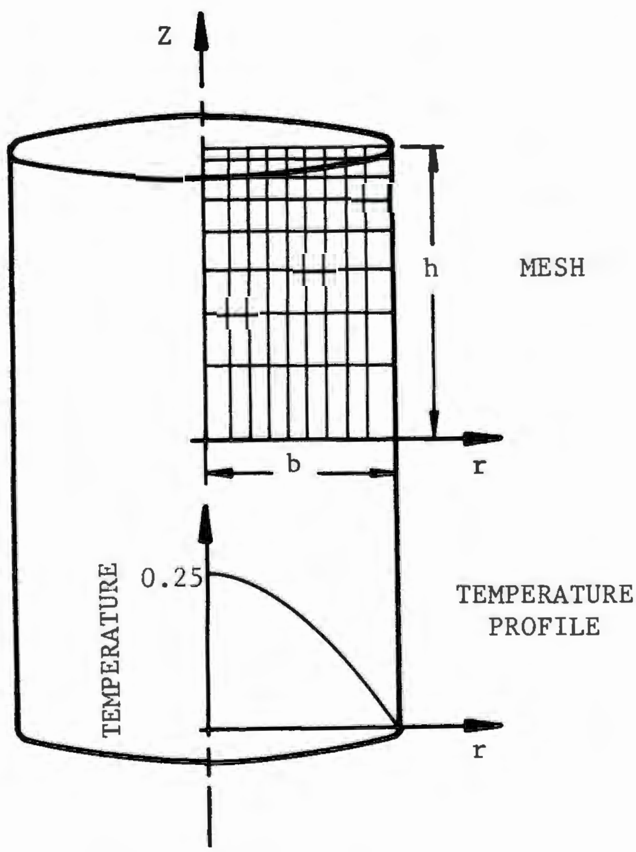


Figure 4.5 Model of cylinder with internal heat generation

Solutions to the deformation and stress fields for this problem are compared with those of Valentin and Carey[31]. The results are calculated in dimensionless terms defined by

$$[u_z \;\; u_r]^T = \frac{-b^3 \alpha Q (1+\nu)}{4k \; (1-\nu)} \; [\hat{u}_z \;\; \hat{u}_r]^T$$

$$\sigma_{ij} = \frac{b^2 \alpha E Q}{4k(1-\nu)} \hat{\sigma}_{ij}$$

where u and σ are the dimensionless variables.
Figure 4.7 shows the deformed shape for cylinders with aspect ratios of 0.5, 1.0 and 2.0 and ν = 0.25. Figures 4.8, 4.9 and 4.10 show the variation along the length of a cylinder of aspect ratio 2.0 of the radial, hoop and axial stresses. Again excellent correlation between the numerical and analytical results is shown in all cases.

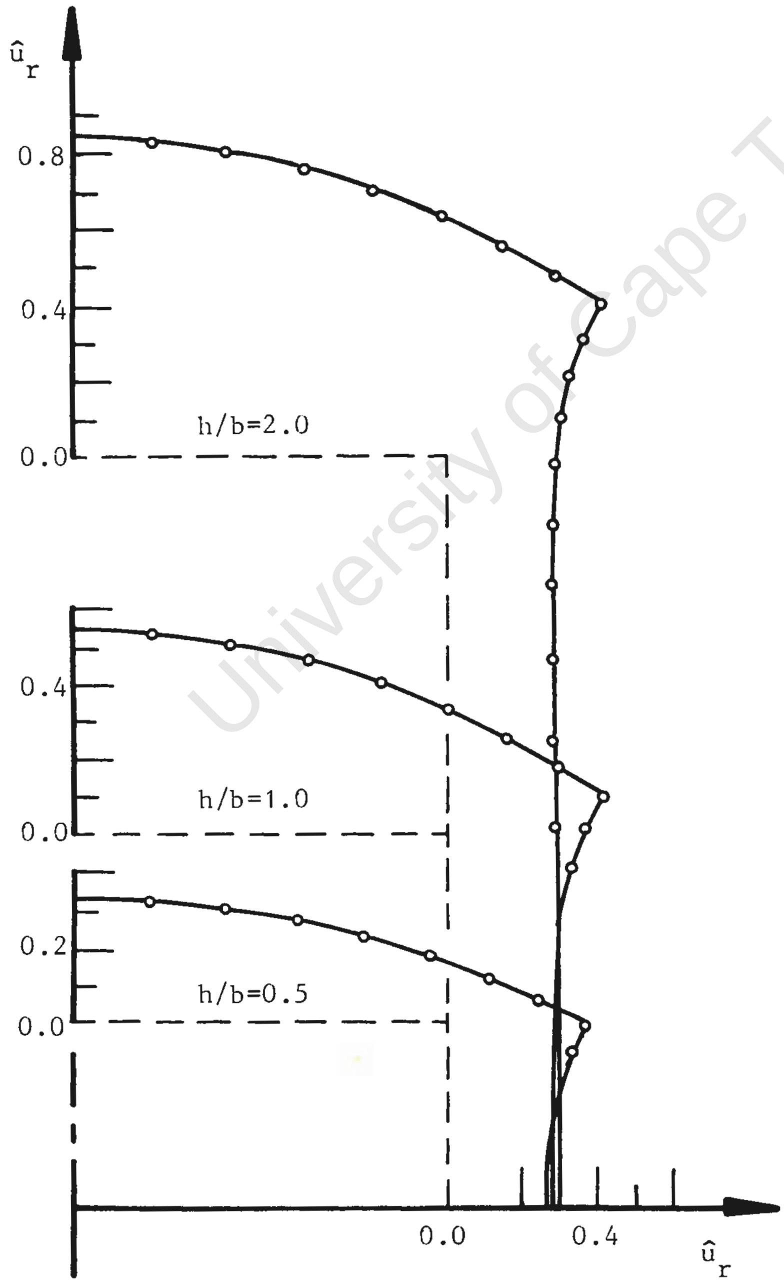


Figure 4.7 Deformation of heat generating cylinders

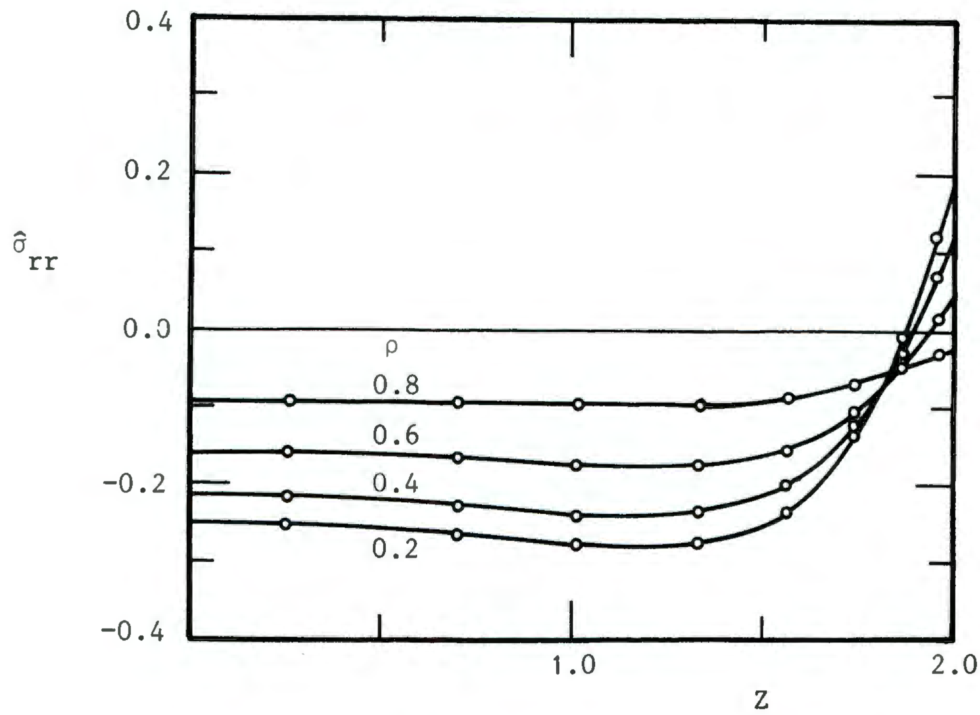


Figure 4.8 Radial stress component as a function of axial position for various values of radius.

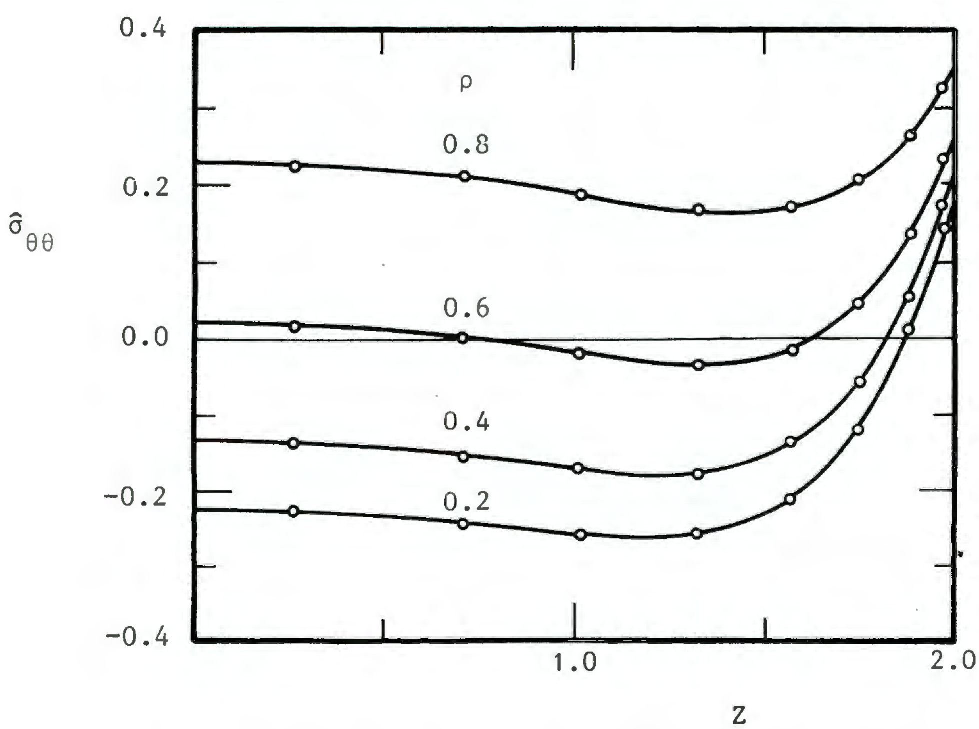


Figure 4.9 Hoop stress component as a function of axial position for various values of radius.

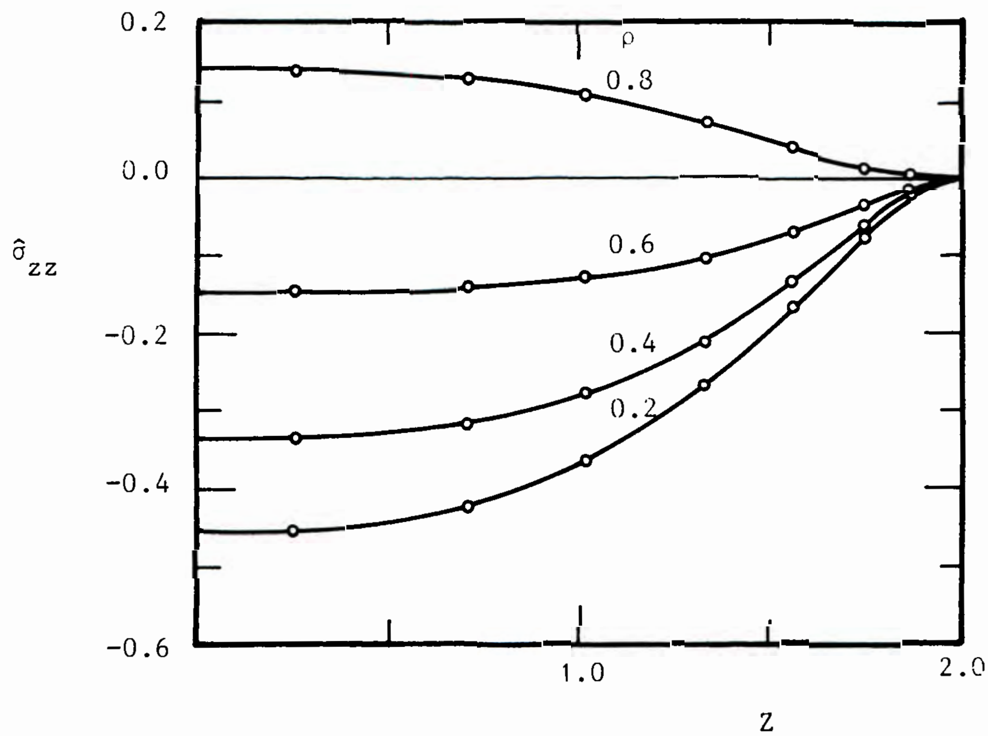


Figure 4.10 Axial stress component as a function of axial position for various values of radius.

CHAPTER FIVE

CONCLUSIONS AND RECOMMENDATIONS

This thesis has considered a finite element approach to the solution of heat transfer and thermo-mechanical stress analysis problems. The development of the steady state equations leads to an uncoupled formulation in which the heat transfer domain is determined prior to and independent of the stress field.

A finite element formulation for the computation of steady state temperature fields in solids with surface heat transfer has been presented. This has been implemented in the mechanical stress analysis code, NOSTRUM[1] such that the thermal strains resulting from the temperature field lead to determination of the stress fields. The principles behind the finite element method used are well established and as such were not expanded or verified with empirical findings. Rather, the numerical procedures developed were compared with analytical solutions to standard problems. The examples presented do not therefore exhibit the modelling abilities of the methods but illustrate the success of the implementation.

During its development, the implementation was also compared with the finite element code, ABAQUS[28]. In all the purely heat transfer problems compared, almost perfect correlation was found. Any small differences were attributed to the different convergence tests used in ABAQUS and NOSTRUM, since these differences could be "eliminated" by applying very stringent convergence criteria.

However, for thermo-mechanical analyses, the two codes have different formulations. ABAQUS has been developed for the fully coupled case so that iterations over the combined mechanical and thermal computations are required. The elements used interpolate to one order higher for geometry and displacement than for temperature. The lower order temperature interpolation is chosen to give the same interpolation order for thermal strain (which is proportional to temperature) as for total strain. This is so that the thermal strain residuals have the same order as the actual load input and can be incorporated in the nonlinear solution procedure.

However, for the uncoupled case developed here, it is consistent to apply thermal strains of the same order as the displacement interpolation order. This is because these strains are merely used in the calculation of equivalent nodal loads, and not in the determination of residuals for the iterative procedure in nonlinear problems. This enables better approximated temperature fields to be applied for general meshes, though in the limit, as the mesh is refined, the same solution is achieved.

The nonlinearities which NOSTRUM/THERMAL has been programmed to deal with are temperature dependent conductivity and internal heat generation for the heat transfer mode, and then the various temperature independent plasticity models which have been implemented by other NOSTRUM research workers. This leaves a number of possibilities for further refinement which are recommended.

1. That the nonlinear heat transfer loading be extended to include the boundary conditions of convection and radiation. The implementation of the former amounts in effect to the extension of distributed surface fluxes to include temperature dependence, and can thus be implemented in a manner similar to nonlinear internal heat generation.

   Radiation however, is more complicated. If the incident radiation is from a distance source, it may be dealt with in the same way as specified surface heating, except that the direction of the distant source must be taken into account in determining the projected area actually presented to the source. If the incident radiation is between surfaces, then the geometrical relationship and reflection of energy between the surfaces must be considered. This involves the introduction of a view factor matrix, details of which may be found in ref.[4].

2. That the full or modified Newton- Raphson iteration scheme be implemented through the inclusion of the [ΔC] and [ΔR] terms into the Jacobian matrix. This also requires that a non symmetric equation solver be used.

3. That the facility for temperature dependence of the mechanical properties such as Poissons ratio, Youngs modulus and coefficient of expansion be introduced. This could be achieved along lines very similar to those used in NOSTRUM/THERMAL for evaluation of the conductivity matrix [k], where in the mechanical case updated values of E and ν could be used in calculating the elasticity matrix [D].

4. That the pure heat transfer mode be documented in a manual in such a way that it can be used for more than just the quasi-harmonic heat transfer equation. In other words, that the input be suitably adjusted so

that the programme can be used to solve problems such as torsion and diffusion, as listed in table 1.1.

These recommendations are all for the steady state case. The extension to the transient or dynamic cases is also a logical step, but since that involves a different starting equation for heat transfer, and further complications in the programming for NOSTRUM/THERMAL as it stands, this is only proffered with caution.

CHAPTER SIX

REFERENCES

1. DUFFETT, G.A., GRIFFIN, T.B., MARTIN, J.B., MERCER, C.D., REDDY, B.D. & RESENDE, L.
NOSTRUM - A Finite Element Program for Nonlinear Structural Mechanics. - Report 18b - Applied Mechanics Research Unit University of Cape Town, 1983.

2. ZIENKIEWICZ, O.C.
"The Finite Element Method in Engineering Science", McGraw Hill - London, 1971.

3. RAO, S.S.
"The Finite Element Method in Engineering" - Pergamon Press (1982).

4. HUEBNER, K.H. & THORNTON, E.A.
"The Finite Element Method for Engineers" - 2nd Ed., John Wiley & Sons (1982).

5. ODEN J.T.
"A General Theory of Finite Elements II Applications" Int. J. Numer. Methods Eng., Vol.1 No.2, (1969).

6. WILSON, E.L., BATHE, K.J., PETERSEN, F.E.,
"Finite Element Analysis of Linear and Nonlinear Heat Transfer", Nuc. Eng. Des. 29 (1974) pp. 110-124.

7. ODEN, J.T. & KROSS, D.A.
"Analysis of General Coupled Thermoelasticity Problems by the Finite Element Method" - Proc. Second Conf. on Matrix Methods in Structural Mech., Report AFFDL-TR-68-150, Wright-Patterson, A.F. Base Ohio (1969) pp 1091-1120.

8. MERIC, R.A.,
"Finite Element Analysis of Optimal Heating of Slab with Temperature Dependent Thermal Conductivity". Int. J. Heat Mass Transfer. Vol. 22 (1979) pp 1347-1353.

9. LEELAMMA MANI & SHUKLA, K.N..
"Application of Finite Element Method to Nonlinear Heat Condition Problems". Numerical Methods for Coupled Problems - eds. Hinton, E., Bettess, P & Lewis R.W. - Procs. of Int. Conf. held at the University College, Swansea, Pineridge Press.
7-11 Sept. (1981) .

10. LYNESS, J.F., OWEN, D.R.J. & ZIENKIEWICZ, O.C.
"The Finite Element Analysis of Engineering Systems Governed by a Nonlinear Quasi-Harmonic Equation". Comput Struct, Vol. 5 (1975) pp 65-79.

11. HAYS, D.F. & CURD, H.N.
Heat Conduction in Solids - Temperature Dependent Thermal Conductivity. Int. J. Heat Mass Transfer Vol. 11 (1968) pp 285-295.

12. PADOVAN, J.
"Steady Conduction of Heat in Linear and Nonlinear Fully Anisotropic Media by Finite Elements". J. Heat Transfer, August (1974) pp 313-317

13. BATHE, K.J. & KHOSHGOFTAAR, M.R.,
"Finite Element Formulation and Solution of Nonlinear Heat Transfer", Nuc. Eng. Des.51 (1979) pp. 389-201.

14. REDDY, B.S. & SHARAN, A.M.
The Transcient Heat Transfer Analysis of Solids with Radiative Boundary Conditions using Finite Element Analysis. Int. Comm. Heat Mass Transfer, Vol. 12 No.2 (1985) pp 169-178.

15. THORNTON, E.A. & WIETING, A.R.,
"A Finite Element Thermal Analysis Procedure for Several Temperature Dependent Parameters", J. Heat Transfer, Vol 100, August (1978), pp. 551-553.

16. HUGHES, T.J.R.,
"Unconditionally Stable Algorithms for Nonlinear Heat Conduction". Comput. Methods Appl. Mech. Eng. 10 (1977) pp 135-139.

17. BIOT, M.A.
"Thermo Elasticity and Irreversible Thermodynamics". J. Appl. Physics Vol 27, No.3 March (1956) pp 240-253

18. KERAMIDAS, G.A. & TING, E.C.
"A Finite Element Formulation for Thermal Stress Analysis, Part I : Variational Formulation", Nuc. Eng. Des. 39 (1976) pp. 267-275.

19. KERAMIDAS, G.A. & TING, E.C.,
"A Finite Element Formulation for Thermal Stress Analysis, Part II : Finite Element Formulation", Nuc. Eng. Des. 39 (1976) pp. 277-287.

20. ZUDANS, Z., YEN, T.C. & STEIGELMANN, W.H.
"Thermal Stress Techniques in the Nuclear Industry" - The Franklin Insitute Research Laboratories, New York (1965).

21. BATHE, K.J.
"Finite Element Procedures in Engineering Analysis" - Prentice Hall, Inc., New Jersey (1982).

22. OWEN, D.R.J. & HINTON, E.
"Finite Elements in Plasticity : Theory and Practice" - Pineridge Press, Swansea, UK.(1980)

23. GRILL, A. & SORIMACHI, K.
"The Thermal Loads in the Finite Element Analysis of Elasto-Plastic Stresses." Int. J. Numer. Methods Eng., Vol. 14 (1979) pp 499-505.

24. WU, C.H.
"Plane Anisotropic Thermoelasticity". J.Appl. Mech., Vol. 51 December (1984), pp 724-726.

25. HINTON, E. & OWEN, D.R.J.
"Finite Element Programming" - Academic Press, London (1977).

26. HIBBITT, KARLSSON & SORENSEN,
ABAQUS Users Manual, Version 4, July (1982).

27. NOSTRUM Users Manual, Applied Mechanics Research Unit/CSIR, University of Cape Town (1985)

28. NOSTRUM Theoretical Manual, Nonlinear Structural Mechanics Research Unit, University of Cape Town, Version 2.1, February (1982).

29. DONEA, J. & GIULIANI, S.
"Finite Element Analysis of Steady State Nonlinear Heat Transfer Problems", Nuc. Eng. Des. 30 (1974) pp 205-213.

30. BORESI, A.P.,
"Stress Problem of Contiguous Co-axial Circular Cylinders subjected to Non-Homogeneous Temperature Distribution and to Pressure", Nuc. Eng. Des.1 (1965) pp 186-196.

31. VALENTIN, R. & CAREY, J.
"Thermal Stresses and Displacements in Finite, Heat Generating Circular Cylinders", Nuc. Eng. Des. 12 (1970) pp 277-290.

APPENDIX A

Subroutines for the Conversion of NOSTRUM to NOSTRUM/THERMAL

The subroutines developed in the programming for inclusion of the thermal effects in NOSTRUM are described in this appendix. Where possible the existing format of NOSTRUM was followed, and the standard routines for evaluating isoparametric element conductance matrices and flux vectors by numerical integration were used.

Figure A1 shows the flow chart for the heat transfer mode, as inserted in NOSTRUM. A brief explanation of the various routines is given below:

HTFLUX	Heat Transfer FLUX assembly - controls the assembly of the flux vector according to the heating data specified. For edge heating the relevant element and edge on which heating occurs is located.
INTPOL	INTer POLate - determines the proportion of the flux to be applied for the particular time step according to the incremental heating procedure specified.
EDGEHT	EDGE HeaTing - determines from the edge heating profile specified, the proportion of the flux to be assigned to each "node" in the flux vector.
GAUSSQ	GAUSSian Quadrature subroutine - sets up sampling point positions and weighting factors for numerical integration.
SHAP2D	SHAPe functions for 2 Dimensional continuum finite elements are calculated.

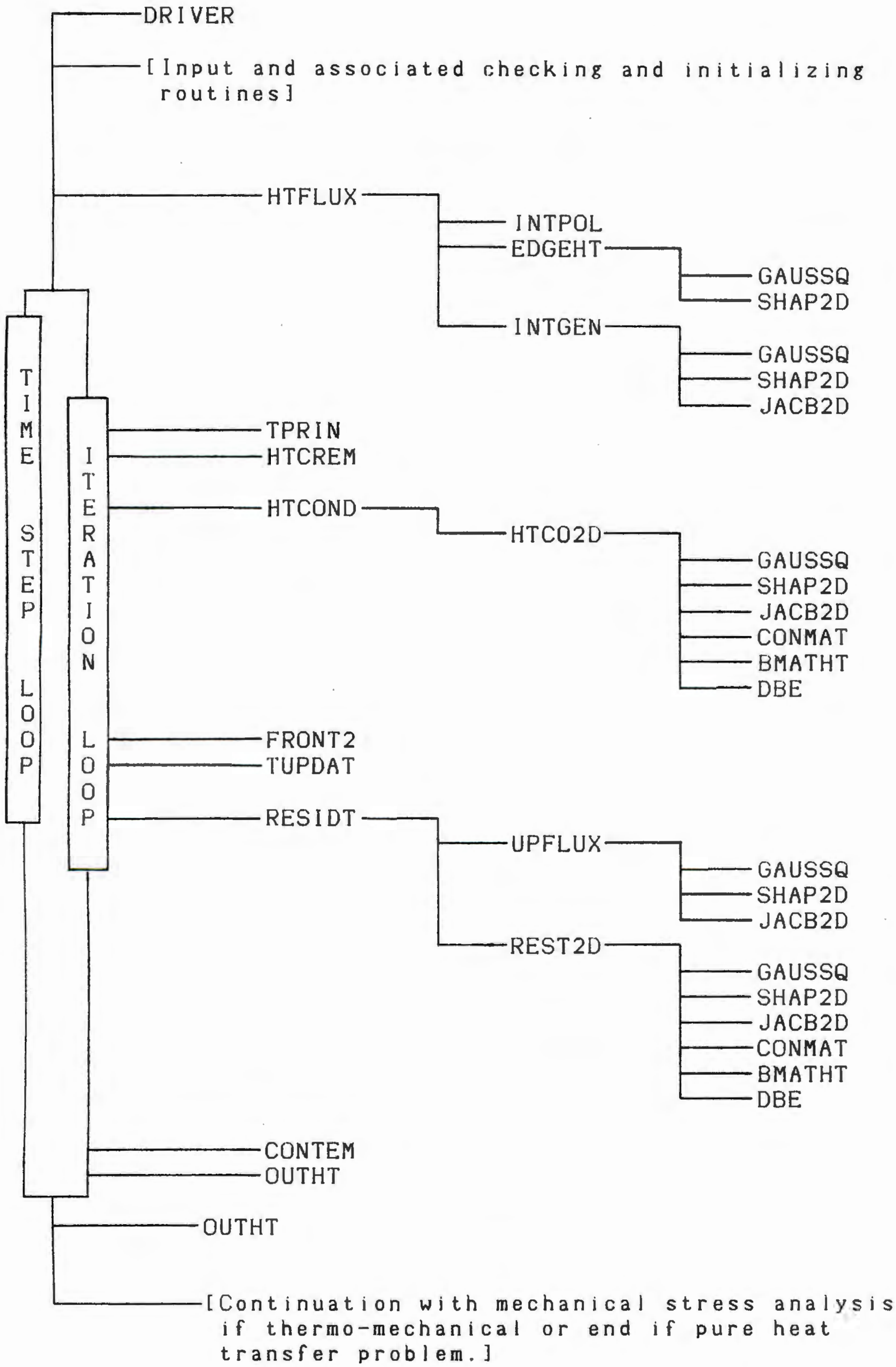


Figure A1: Flow chart of heat transfer section of NOSTRUM/THERMAL

INTGEN	INTernal heat GENeration - integrates the heat generation value of the material over the element volume and determines the proportion of the total heating to be assigned to each node of the element.
JACB2D	JACoBian for 2 Dimensional finite elements - calculates 1) The co-ordinates of the Gauss points 2) the Jacobian matrix 3) the inverse of the Jacobian matrix 4) the Cartesian shape function derivatives.
TPRIN	Time PRINt - determines if output is to be printed for the particular time step.
HTCREM	Heat Transfer flux inCREMent - sets up the current flux step.
HTCOND	Heat Transfer CONDuctance matrix assembly - controls the conductance matrix assembly for each element group.
HTCO2D	Heat Transfer COnductance matrix assembly for 2 Dimensional finite elements - evaluates the conductance matrices due to conductivity alone.
CONMAT	CONductivity MATrix - is evaluated for the current element. (The parallel in stress analysis is the elasticity matrix).
BMATH	B MATrix for Heat transfer - is evaluated.
DBE	product of D and B matrices Evaluated.

FRONT2 FRONTal equation solver 2 - solves for the single degree of freedom per node, temperature, by the frontal method.

TUPDAT Temperature UPDATing routine adds the current temperature increments to the total temperatures and includes the current reaction flux increments in the total flux array.

UPFLUX UPdate FLUX vector - accounts for any dependence of internal heat generation on temperature and incorporates this into the total flux vector.

RESIDT RESIDual heat Transfer subroutine - controls the calculation of internal flux due to the new temperature field.

REST2D RESidual heaT flux for 2 Dimensional continuum elements - calculates the equivalent nodal flux imbalance due to the affect the new temperature field has on temperature dependent conductivity. If conductivity is unaffected by temperature then fluxes calculated will have the same values as those initially imposed on the system, and any convergence criterion will be satisfied.

CONTEM CONvergence of TEMperatures tested for nonlinear heat transfer.

OUTHT OUTput of Heat Transfer results.

The inclusion of thermal deformation effects in NOSTRUM resulted in changes to the temperature independent program in the following subroutines.

DRIVER The DRIVER of NOSTRUM is expanded to include control of the heat transfer solution mode.

INPUT	Data related to the control of the thermal aspects, thermal material properties and boundary conditions are collected by the input routine.
PROCED	Common blocks for the thermal problems are included.
CHCTRL	CHeck ConTRoL includes code for checking the thermal control data.
WARN	WARNing messages are included for the thermal aspect.
DOFRON	Sets up global Degree Of Freedom numbering and calculates the maximum fRONt width required for both heat transfer and mechanical analysis frontal solution.
READEG	READs Element Group data
LOADS	controls the assembly of the mechanical load vector including thermal strain loads.
INSLD2	is called by LOADS to calculate the INitial Strain nodal Loads for 2 Dimensional problems due to imposed and thermal strains.
RESD2D	computes RESiDual nodal forces for 2 Dimensional elements once thermal or initial strains have been excluded.
LINEAR	computes the stresses for LINEAR elastic deformation includes the z components and E α T for the plane strain assumption.

APPENDIX B

Course Work

In compliance with the requirements for the Masters Degree, approved course work with a value of twenty one credits was done in addition to the thesis. These courses are briefly described below.

(i) CE5B7 - **Introduction to the Theory of Elasticity.**
Stress, strain, equilibrium strain displacement relations. Elastic constants. Solutions of simple boundary value problems in plane stress and plane strains.
(2 credits)

(ii) CE5B8 - **Plates and Shells**
An introduction to the elastic theory of plates and shells. Generalised stresses, generalised strains, elastic constitive relations, coordinate systems. Analytical solutions of simple problems.
(2 credits)

(iii) CE5B9 - **Introduction to the Finite Element Method**
Generalised displacement method of analysis for framed structures. Elastic energy theorems. Basic procedures of the finite element method illustrated for frame structures.
(2 credits)

(iv) **CE5B10 - Finite Element Analysis**

Plane stress and plane strain elements, plate bending elements, shell elements, three-dimensional elements. Programming of the finite element displacement method. Techniques for equation solving.

(3 credits)

(v) **AM343 - Numerical Analysis**

An introduction to theory and practice in a wide range of numerical methods. The approximate solution of non-linear equations. Interpolation and approximation. Numerical differentiation and integration. Numerical solution of ordinary differential equations. Numerical solution of simultaneous linear equation. Approximation function. Eigenvalue methods.

(4 credits)

(vi) **AM344 - Advanced Numerical Analysis**

Introduction to the finite element method for partial differential equations.

(4 credits)

(vii) **AM367 - Continuum Mechanics**

Introduction to the mathematical treatment of fluid mechanics and elasticity. Fluid and solid mechanics, Novier-Stokes eequations, the partial differential equations of elasticity.

(3 credits)