39
6/30/80 T.S.
Special Distribution

WAPD-TM-1384
DOE RESEARCH AND
DEVELOPMENT REPORT

FINITE DEFORMATION ANALYSIS OF CONTINUUM STRUCTURES WITH TIME DEPENDENT ANISOTROPIC ELASTIC PLASTIC MATERIAL BEHAVIOR

(LWBR/AWBA Development Program)

D. N. Hutula

MARCH 1980

CONTRACT DE-AC11-76PN00014

BETTIS ATOMIC POWER LABORATORY
WEST MIFFLIN, PENNSYLVANIA

Operated for the U. S. Department of Energy by
WESTINGHOUSE ELECTRIC CORPORATION

DISCLAIMER

WAPD-TM-1384

Master

FINITE DEFORMATION ANALYSIS OF CONTINUUM STRUCTURES WITH TIME-DEPENDENT ANISOTROPIC ELASTIC-PLASTIC MATERIAL BEHAVIOR

(LWBR/AWBA Development Program)

David N. Hutula

March 1980

Contract Number DE-AC11-76PN00014

Printed in the United States of America
Available from the
National Technical Information Service
U. S. Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22151

NOTE

This document is an interim memorandum prepared primarily for internal reference and does not represent a final expression of the opinion of Westinghouse. When this memorandum is distributed externally, it is with the express understanding that Westinghouse makes no representation as to completeness, accuracy, or usability of information contained therein.

BETTIS ATOMIC POWER LABORATORY WEST MIFFLIN, PENNSYLVANIA 15122

Operated for the U.S. Department of Energy
by WESTINGHOUSE ELECTRIC CORPORATION

FOREWORD

The Shippingport Atomic Power Station located in Shippingport, Pennsylvania was the first large-scale, central-station nuclear power plant in the United States and the first plant of such size in the world operated solely to produce electric power. This program was started in 1953 to confirm the practical application of nuclear power for large-scale electric power generation. It has provided much of the technology being used for design and operation of the commercial, central-station nuclear power plants now in use.

Subsequent to development and successful operation of the Pressurized Water Reactor in the DOE-owned reactor plant at the Shippingport Atomic Power Station, the Atomic Energy Commission in 1965 undertook a research and development program to design and build a Light Water Breeder Reactor core for operation in the Shippingport Station.

The objective of the Light Water Breeder Reactor (LWBR) program has been to develop a technology that would significantly improve the utilization of the nation's nuclear fuel resources employing the well-established water reactor technology. To achieve this objective, work has been directed toward analysis, design, component tests, and fabrication of a water-cooled, thorium oxide fuel cycle breeder reactor for installation and operation at the Shippingport Station. The LWBR core started operation in the Shippingport Station in the Fall of 1977 and is expected to be operated for about 3 to 4 years. At the end of this period, the core will be removed and the spent fuel shipped to the Naval Reactors Expended Core Facility for a detailed examination to verify core performance including an evaluation of breeding characteristics.

In 1976, with fabrication of the Shippingport LWBR core nearing completion, the Energy Research and Development Administration established the Advanced Water Breeder Applications (AWBA) program to develop and disseminate technical information which would assist U. S. industry in evaluating the LWBR concept for commercial-scale applications. The program will explore some of the problems that would be faced by industry in adapting technology confirmed in the LWBR program. Information to be developed includes concepts for commercial-scale prebreeder cores which would produce uranium-233 for light water breeder cores while producing electric power, improvements for breeder cores based on the technology developed to fabricate and operate the Shippingport LWBR core, and other information and technology to aid in evaluating commercial-scale application of the LWBR concept.

All three development programs (Pressurized Water Reactor, Light Water Breeder Reactor, and Advanced Water Breeder Applications) have been administered by the Division of Naval Reactors with the goal of developing practical improvements in the utilization of nuclear fuel resources for generation of electircal energy using water-cooled nuclear reactors.

Technical information developed under the Shippingport, LWBR, and AWBA programs has been and will continue to be published in technical memoranda, one of which is this present report.

CONTENTS

NOTATION

C_{IJKL} : Compliance tensor. See Equation (3.11).

C^{e}_{IJKL} : Elastic compliance tensor. See Equation (3.4).

C^{po}_{IJKL} : Plastic compliance tensor. See Equation (3.8).

D^{IJKL} : Stiffness tensor. See Equation (3.12).

D^{ijkl} : Stiffness tensor. See Equation (3.28).

D^{ijkl}_{*} : See Equation (3.30).

$\bar{e}_I$: Unit base vector of characteristic axis I. See Equation (3.1).

e^{ijk}, e_{ijk} : Permutation symbol. See Equation (2.6) and discussion following.

$\bar{F}$: Body force vector per unit mass. See Equation (4.5).

f^i : Contravariant component of $\bar{F}$. See Equation (4.5).

$\Delta f^{i\alpha}$: Nodal force increment. See Equation (5.4).

$\Delta f^{i\alpha}_{p}$: Nodal force increment due to pressure loads. See Equation (5.5).

$\Delta f^{i\alpha}_{B}$: Nodal force increment due to body force. See Equation (5.5).

$\Delta f^{i\alpha}_{*}$: Nodal force increment due to plastic and growth strain increments. See Equation (5.5).

$f^{i\alpha}_{R}$: Residual nodal force. See Equation (5.6).

$\bar{g}_i$, $\bar{g}^i$: Covariant and contravariant base vectors of θ^i coordinate system at time t_o. See Equations (2.3a) and (2.6a).

g_{ij}, g^{ij}, g^i_j : Covariant, contravariant, and mixed metric tensors of θ^i coordinate system at time t_o. See Equations (2.4a), (2.7a), and (2.8a).

g : Determinant of g_{ij}.

$\bar{G}_i$, $\bar{G}^i$: Covariant and contravariant base vectors of θ^i coordinate system at time t. See Equations (2.3b) and (2.5b).

G_{ij}, G^{ij}, G^i_J : Covariant, contravariant, and mixed metric tensors of θ^i coordinate system at time t. See Equations (2.4b), (2.7b), and (2.8b).

G : Determinant of G_{ij}.

$[G]$	:	3x3 matrix whose elements are G_{ij}.
$\bar{i}_j$	:	Unit base vector of Cartesian coordinate system
$[I]$	:	3x3 unit matrix.
J	:	Volume ratio. See Equations (2.18) and (2.19).
$K^{i\alpha j\beta}$	:	Finite element stiffness matrix. See Equation (5.3).
$\bar{n}$	:	Unit vector normal to a surface at time t_o.
n_i	:	Covariant component of $\bar{n}$.
$\bar{N}$	:	Unit vector normal to a surface at time t.
N_i	:	Covariant component of $\bar{N}$.
N^α	:	Isoparametric finite element shape function associated with node α. See Equation (5.1).
o	:	Subscript or superscript used to denote quantity evaluated at time t_o.
p	:	Pressure
q_I^i	:	Transformation tensor relating $\bar{g}_i$ to $\bar{e}_I$. See Equation (3.1).
Q_I^i	:	Transformation tensor relating $\bar{G}_i$ to $\bar{e}_I$. See Equation (3.1).
$[Q]$	:	3x3 matrix whose elements are Q_I^i, where i is the row index and I is the column index.
$\bar{r}$, $\bar{R}$	:	Position vector of a material point at time t_o and t, respectively. (See Equation (2.2).
S	:	Surface.
S_p	:	Surface over which pressure is applied.
t	:	Time.
t_o	:	Time at beginning of a time step.
$\bar{T}$	:	Traction or stress vector acting on a surface. See Equations (2.17) and (4.6).
$\Delta\bar{u}$	:	Displacement increment vector. See Equation (2.9).
$\Delta u_i, \Delta u^i$	:	Covariant and contravariant components of $\Delta\bar{u}$. See Equation (2.9).

$\Delta u_{i\alpha}$: Δu_i at node α. See Equation (5.1).

$\bar{v}$: Velocity vector. See Equation (2.10).

v_i, v^i : Covariant and contravariant components of $\bar{v}$. See Equation (2.10).

V : Volume.

x_i, X_i : Cartesian coordinates of a material point at time t_o and t, respectively.

$x_{i\alpha}, X_{i\alpha}$: x_i and X_i at node α. See Equation (5.1).

$\dot{\gamma}_{ij}$: Strain rate or deformation rate tensor defined by Equation (2.14).

$\Delta\gamma_{ij}$: Strain increment from t_o to t defined by Equation (2.15).

$[\Delta\gamma]$: 3x3 matrix whose elements are $\Delta\gamma_{ij}$.

δ_i^j : Kronecker delta. See Equation (2.8).

$\dot{\epsilon}_{IJ}$: Strain rate or deformation rate tensor defined by Equation (3.2).

$\dot{\epsilon}^e_{IJ}$: Elastic strain rate. See Equation (3.3).

$\dot{\epsilon}^p_{IJ}$: Plastic strain rate. See Equation (3.3).

$\dot{\epsilon}^g_{IJ}$: Growth strain rate. See Equation (3.3).

$\Delta\epsilon_{IJ}$: Strain increment from t_o to t defined by Equation (3.24).

$[\Delta\epsilon]$: 3x3 matrix whose elements are $\Delta\epsilon_{IJ}$.

$\Delta\epsilon^*_{IJ}$: Defined by Equation (3.11).

$\Delta\epsilon^{p_o}_{IJ}$: Defined by Equation (3.8).

θ^i : Curvilinear material coordinate defined in Section 2.

$[\lambda]$: 3x3 diagonal matrix of eigenvalues of [G]. See Equation (3.20).

ρ_o, ρ : Density at time t_o and t.

σ^{IJ} : Stress tensor defined by Equation (3.2).

$\dot{\sigma}^{IJ}$: Stress rate tensor. Time derivative of σ^{IJ}.

$\Delta \sigma^{IJ}$	:	Stress increment from t_o to t.
$\Delta \sigma^{IJ}_*$	:	Defined by Equation (3.13).
τ^{ij}	:	Stress tensor defined by Equation (2.17).
τ^{ij}_*	:	Defined by Equation (3.28).
$\Delta\tau^{ij}_*$	:	Defined by Equation (3.28).
$[\varphi]$	:	3x3 orthogonal matrix of eigenvectors of [G]. See Equation (3.20).
$\overline{\omega}$	:	Vorticity or spin vector. See Equation (2.16).
$\dot{(\ )}$	:	Derivative of ( ) with respect to time.
$(\ )_{,i}$	:	Partial derivative of ( ) with respect to θ^i.
$(\ )_{;i}$	:	Covariant derivative ( ) with respect to θ^i, evaluated using g_{ij} metric tensor.
$(\ )_o$, $(\ )^o$	:	The quantity ( ) evaluated at time t_o.
$\delta\ (\ )$	:	Variation or virtual change in the quantity ( ).
$\Delta\ (\ )$	:	Increment in the quantity ( ) from t_o to t.

ABSTRACT

A finite element procedure is presented for finite deformation analysis of continuum structures with time-dependent anisotropic elastic-plastic material behavior. An updated Lagrangian formulation is used to describe the kinematics of deformation. Anisotropic constitutive relations are referred, at each material point, to a set of three mutually orthogonal axes which rotate as a unit with an angular velocity equal to the spin at the point. The time-history of the solution is generated by using a linear incremental procedure with residual force correction, along with an automatic time step control algorithm which chooses time step sizes to control the accuracy and numerical stability of the solution.

FINITE DEFORMATION ANALYSIS OF CONTINUUM STRUCTURES WITH TIME-DEPENDENT ANISOTROPIC ELASTIC-PLASTIC MATERIAL BEHAVIOR

(LWBR/AWBA Development Program)

David N. Hutula

1. INTRODUCTION

Detailed design evaluation of structural components which must maintain structural integrity over long periods of time under severe loading and environmental conditions requires an analysis method which characterizes the actual behavior by accurately modelling the significant behavioral phenomena. The three basic ingredients of such an analysis method are accurate modelling of the material behavior, accurate modelling of the geometry (including the effects of finite changes in geometry due to deformation), and an effective numerical procedure for solving the mathematical equations of the model.

The analysis method or procedure presented in this document is designed to handle problems involving finite deformation of continuum structures with time-dependent anisotropic elastic-plastic material behavior. In order to allow its implementation in a digital computer program, the procedure employs

the finite element method to establish a spatially discretized form of the governing equations. A linear incremental formulation with residual force correction and automatic time step control is used to generate the time-history of the solution. The kinematics of deformation are described by using an updated Lagrangian formulation in which the configuration at the beginning of each time step serves as the Lagrangian frame of reference for that time step.

A unique feature of the analysis method or procedure is an automatic time step control algorithm which chooses time step sizes to control the accuracy and numerical stability of the solution. This feature makes the solution of finite deformation elastic-plastic problems almost routine and allows the structural analyst to concentrate on the physical aspects of a problem without being overburdened by the intricacies of the numerical analysis.

Another unique feature is the treatment of "characteristic axes" to which anisotropic constitutive relations are referred. The characteristic axes in the formulation are, at each material point, three mutually orthogonal axes which rotate as a unit as the material in the neighborhood of the point deforms and rotates. A procedure is derived for keeping track of the instantaneous orientation of the characteristic axes relative to a fixed frame of reference.

The analysis procedure has been implemented in the ACCEPT (Analysis of Creep-Collapse of Externally-Pressurized Tubes) computer program described in Reference 1. The effectiveness of the procedure has been demonstrated by extensive numerical experimentation with and production usage of the ACCEPT program.

2. FUNDAMENTAL EQUATIONS AND DEFINITIONS

Fundamental concepts involving coordinate systems, kinematics of deformation, and stress are reviewed in this section. All variables and equations are understood to be associated with a generic material point in a solid continuum. This point is identified by its position vector $\bar{r}$ at some time* t_o and by its position vector $\bar{R}$ at a later time t.

The formulation used here follows that of Green and Zerna (Reference 2), in which a curvilinear coordinate system θ^i whose coordinate lines are imbedded in the material is used to describe the motion of the continuum during the time span from t_o to t. In Green and Zerna's formulation, the curvilinear material coordinates are related to Cartesian coordinates through transformations denoted symbolically as

$$x^j = x^j(\theta^1,\theta^2,\theta^3)$$
$$X^j = X^j(\theta^1,\theta^2,\theta^3) \qquad (2.1a,b)$$

where x^j and X^j are the Cartesian coordinates of a material point at time t_o and t, respectively.

The position vectors of a material point are expressed in terms of Cartesian coordinates as**

$$\bar{r} = x^j\bar{i}_j$$
$$\bar{R} = X^j\bar{i}_j \qquad (2.2a,b)$$

where $\bar{i}_j$ are the mutually orthogonal unit base vectors of the Cartesian coordinate system.

---

* t_o represents the time at the beginning of a time step in the incremental solution procedure formulated in this document.

** The Einstein summation convention applies throughout this document. That is, a repeated index implies a summation over the range of the index.

The covariant base vectors, $\bar{g}_i$ and $\bar{G}_i$, and metric tensors, g_{ij} and G_{ij}, of the θ^i coordinate system at time t_o and t, respectively, are *

$$\bar{g}_i = \bar{r}_{,i} = x^j_{,i}\, \bar{i}_j \qquad (2.3a,b)$$

$$\bar{G}_i = \bar{R}_{,i} = X^j_{,i}\, \bar{i}_j$$

$$g_{ij} = \bar{g}_i \cdot \bar{g}_j \qquad (2.4a,b)$$

$$G_{ij} = \bar{G}_i \cdot \bar{G}_j$$

The contravariant base vectors, $\bar{g}^i$ and $\bar{G}^i$, and metric tensors, g^{ij} and G^{ij} are

$$2\sqrt{g}\, \bar{g}^i = e^{ijk}\, \bar{g}_j \times \bar{g}_k \qquad (2.5a,b)$$

$$2\sqrt{G}\, \bar{G}^i = e^{ijk}\, \bar{G}_j \times \bar{G}_k$$

$$\sqrt{g}\, e_{ijk}\, \bar{g}^i = \bar{g}_j \times \bar{g}_k \qquad (2.6a,b)$$

$$\sqrt{G}\, e_{ijk}\, \bar{G}^i = \bar{G}_j \times \bar{G}_k$$

$$g^{ij} = \bar{g}^i \cdot \bar{g}^j \qquad (2.7a,b)$$

$$G^{ij} = \bar{G}^i \cdot \bar{G}^j$$

where g and G are the determinants of g_{ij} and G_{ij}, respectively, and where e^{ijk} or e_{ijk} is the permutation symbol which is equal to zero when any two of the indices are equal and is equal to +1 (-1) when i,j,k is an even (odd) permutation of the numbers 1, 2, 3.

The covariant base vectors are tangent to the θ^i coordinate lines and the contravariant base vectors are normal to the θ^i coordinate surfaces, as depicted in two dimensions in Figure 1.

---

*Throughout this document, a comma preceding a subscript index i denotes a partial derivative with respect to θ^i. A semicolon denotes a covariant derivative with respect to θ^i evaluated using the g_{ij} metric tensor.

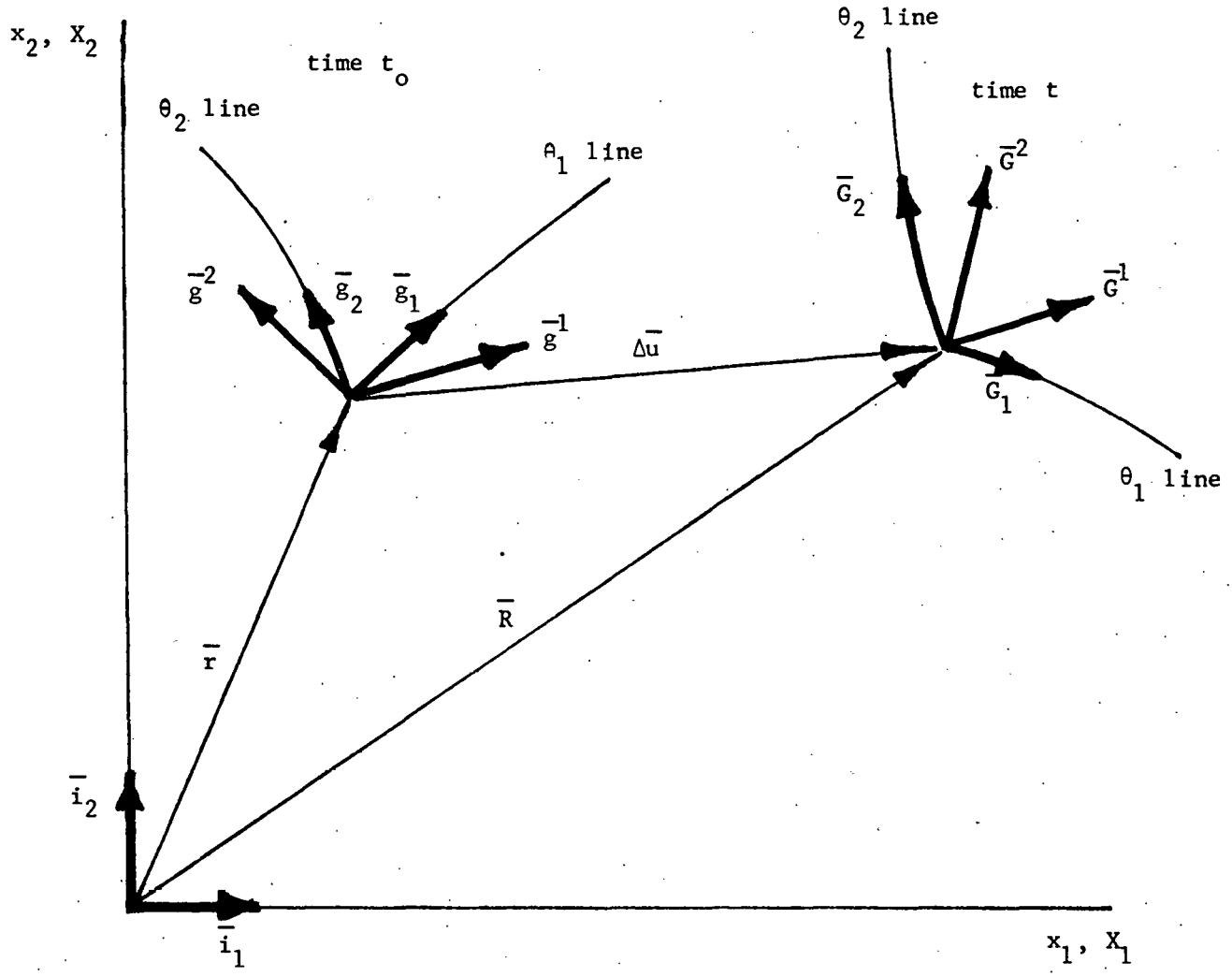

Figure 1: Two-Dimensional Representation of Position Vectors, Incremental Displacement Vector, and Base Vectors.

The contravariant metric tensors are the inverses of the corresponding covariant metric tensors and the contravariant and covariant base vectors satisfy orthogonality relations such that

$$g_{ik}g^{kj} = g_i^j = \bar{g}_i \cdot \bar{g}^j = \delta_i^j$$
$$G_{ik}G^{kj} = G_i^j = \bar{G}_i \cdot \bar{G}^j = \delta_i^j \qquad (2.8a,b)$$

where δ_i^j, the Kronecker delta, is equal to one if i=j and is equal to zero if $i \neq j$.

The increment in the displacement vector from t_o to t and the velocity vector are given by

$$\begin{aligned}\Delta\bar{u} &= \bar{R} - \bar{r} \\ &= \Delta u^i \bar{g}_i = \Delta u_i \bar{g}^i\end{aligned} \qquad (2.9a\text{-}c)$$

$$\begin{aligned}\bar{v} &= \dot{\bar{R}} \\ &= v^i \bar{g}_i = v_i \bar{g}^i\end{aligned} \qquad (2.10a\text{-}c)$$

The partial derivatives of $\Delta\bar{u}$ and $\bar{v}$ with respect to θ^j are

$$\begin{aligned}\Delta\bar{u}_{,j} &= \bar{G}_j - \bar{g}_j \\ &= \Delta u^i_{;j}\bar{g}_i = \Delta u_{i;j}\bar{g}^i\end{aligned} \qquad (2.11a\text{-}c)$$

$$\begin{aligned}\bar{v}_{,j} &= \dot{\bar{G}}_j \\ &= v^i_{;j}\bar{g}_i = v_{i;j}\bar{g}^i\end{aligned} \qquad (2.12a\text{-}c)$$

Equations (2.11), (2.5), and (2.6) can be used to derive the following which relate $\bar{g}_i$ and $\bar{g}^i$ to $\bar{G}_i$ and $\bar{G}^i$ through the displacement gradient increments:

$$\bar{G}_i = (g_i^j + \Delta u^j_{;i})\bar{g}_j$$
$$\bar{G}^i = \tfrac{1}{2}\sqrt{\frac{g}{G}}\, e^{ijk}e_{rst}(g_j^r + \Delta u^r_{;j})(g_k^s + \Delta u^s_{;k})\bar{g}^t \qquad (2.13a,b)$$

The strain rate or deformation rate tensor $\dot{\gamma}_{ij}$ is defined by

$$\begin{aligned}\dot{\gamma}_{ij} &= \tfrac{1}{2}\dot{G}_{ij} \\ &= \tfrac{1}{2}(\dot{\bar{G}}_i \cdot \bar{G}_j + \bar{G}_i \cdot \dot{\bar{G}}_j) \\ &= \tfrac{1}{2}(\bar{v}_{,i} \cdot \bar{G}_j + \bar{G}_i \cdot \bar{v}_{,j}) \\ &= \tfrac{1}{2}[(g_i^k + \Delta u_{;i}^k)v_{k;j} + (g_j^k + \Delta u_{;j}^k)v_{k;i}]\end{aligned} \tag{2.14a-d}$$

The increment in the strain tensor from t_o to t is

$$\begin{aligned}\Delta\gamma_{ij} &= \int_{t_o}^{t} \dot{\gamma}_{ij}\,dt \\ &= \tfrac{1}{2}(G_{ij} - g_{ij}) \\ &= \tfrac{1}{2}(\Delta u_{i;j} + \Delta u_{j;i} + \Delta u_{;i}^k \Delta u_{k;j})\end{aligned} \tag{2.15a-c}$$

The vorticity or spin vector $\bar{\omega}$ is defined to be one-half the curl of the velocity vector field, as follows:

$$\begin{aligned}\bar{\omega} &= \tfrac{1}{2}\bar{\nabla} \times \bar{v} \\ &= \tfrac{1}{2}\bar{G}^i \times \bar{v}_{,i} \\ &= \tfrac{1}{2}\bar{G}^i \times \dot{\bar{G}}_i\end{aligned} \tag{2.16a-c}$$

where $\bar{\nabla} = \bar{G}^i \frac{\partial}{\partial \theta^i}$ is the vector gradient operator.

The stress tensor τ^{ij} is defined as follows in terms of the traction or stress vector $\bar{T}$ acting on an arbitrary infinitesimal surface element whose unit normal vector is $\bar{N} = N_i\bar{G}^i$:

$$\begin{aligned}\bar{T} &= T^j\bar{G}_j \\ &= \tau^{ij}N_i\bar{G}_j\end{aligned} \tag{2.17a,b}$$

τ^{ij} is the contravariant Cauchy or true stress tensor with components referred to the $\bar{G}_i$ base vectors. τ^{ij} and $\dot{\gamma}_{ij}$ are conjugate in the sense that $\tau^{ij}\dot{\gamma}_{ij}$ is the internal work rate per unit volume.

The transformation relating an infinitesimal material volume element dV_o at time t_o to the corresponding element dV at time t can be derived as follows: Consider the three infinitesimal vectors $d\theta^1\bar{g}_1$, $d\theta^2\bar{g}_2$, and $d\theta^3\bar{g}_3$ which emanate from a material point in the continuum at time t_o. These vectors form three intersecting edges of an infinitesimal parallelepiped whose volume is

$$\begin{aligned} dV_o &= [(d\theta^1\bar{g}_1) \times (d\theta^2\bar{g}_2)] \cdot (d\theta^3\bar{g}_3) \\ &= [(\bar{g}_1 \times \bar{g}_2) \cdot \bar{g}_3] d\theta^1 d\theta^2 d\theta^3 \\ &= \sqrt{g}\, d\theta^1 d\theta^2 d\theta^3 \end{aligned}$$

where Equations (2.5a) and (2.8a) were used to derive the final result. At time t, the three vectors described above become $d\theta^1\bar{G}_1$, $d\theta^2\bar{G}_2$, and $d\theta^3\bar{G}_3$ and the corresponding volume is

$$dV = \sqrt{G}\, d\theta^1 d\theta^2 d\theta^3$$

Also, because of conservation of mass, $\rho_o dV_o = \rho dV$. Therefore, the volume transformation relation can be written as

$$\begin{aligned} dV &= \sqrt{\frac{G}{g}}\, dV_o \\ &= \frac{\rho_o}{\rho}\, dV_o \\ &= J dV_o \end{aligned} \qquad (2.18a\text{-}c)$$

Equations (2.8) and (2.13) can be used to derive an expression for the volume ratio $J = \sqrt{\frac{G}{g}}$ in terms of the displacement gradient increments as follows:

$$\begin{aligned} J &= \frac{1}{6} e^{ijk} e_{rst} (g_i^r + \Delta u^r_{;i})(g_j^s + \Delta u^s_{;j})(g_k^t + \Delta u^t_{;k}) \\ &= 1 + \Delta u^i_{;i} + \tfrac{1}{2}\Delta u^i_{;i}\Delta u^j_{;j} - \tfrac{1}{2}\Delta u^i_{;j}\Delta u^j_{;i} \\ &\quad + \frac{1}{6} e^{ijk} e_{rst} \Delta u^r_{;i}\Delta u^s_{;j}\Delta u^t_{;k} \end{aligned} \qquad (2.19a,b)$$

The transformation relating an infinitesimal material surface element at time t_o to the corresponding surface element at time t can be derived as follows: Consider two arbitrary but distinct infinitesimal vectors $d\bar{\ell}_1 = \bar{g}_i d\theta^i_{(1)}$ and $d\bar{\ell}_2 = \bar{g}_j d\theta^j_{(2)}$ emanating from a material point in the continuum at time t_o. These vectors form two edges of an infinitesimal parallelogram whose area dS_o and unit normal vector $\bar{n} = n_k \bar{g}^k$ can be expressed as

$$\begin{aligned}
\bar{n} dS_o &= (n_k dS_o)\bar{g}^k \\
&= d\bar{\ell}_1 \times d\bar{\ell}_2 \\
&= (\bar{g}_i \times \bar{g}_j) d\theta^i_{(1)} d\theta^j_{(2)} \\
&= (\sqrt{g}\, e_{ijk} d\theta^i_{(1)} d\theta^j_{(2)})\bar{g}^k
\end{aligned}$$

Therefore:

$$n_k dS_o = \sqrt{g}\, e_{ijk} d\theta^i_{(1)} d\theta^j_{(2)}$$

At time t, the two vectors described above become $d\bar{L}_1 = G_i d\theta^i_{(1)}$ and $d\bar{L}_2 = \bar{G}_j d\theta^j_{(2)}$. The corresponding infinitesimal parallelogram has an area dS and a unit normal vector $\bar{N} = N_k \bar{G}^k$ such that

$$N_k dS = \sqrt{G}\, e_{ijk} d\theta^i_{(1)} d\theta^j_{(2)}$$

This expression along with the previous one results in the following surface transformation relation:

$$\begin{aligned}
N_k dS &= \sqrt{\frac{G}{g}}\, n_k dS_o \\
&= J n_k dS_o
\end{aligned} \qquad (2.20a,b)$$

The fundamental equations and definitions given in this section will be used in the sections which follow to develop the incremental solution procedure. In all developments which follow, the θ^i coordinate system will be redefined at the beginning of each time step such that the $\bar{g}_i$ base vectors coincide

with the Cartesian $\bar{i}_i$ base vectors. Thus, g_{ij} and g^{ij} are each to be interpreted as the unit tensor, the covariant derivatives such as $\Delta u_{i;j}$ are to be interpreted as partial derivatives with respect to x^j. This formulation, wherein a new Lagrangian frame of reference is defined at the beginning of each time step, is known as an updated Lagrangian formulation.

A consequence of redefining the θ^i coordinate system at the beginning of each time step should be noted regarding the interpretation of $\Delta\gamma_{ij}$. The increments $\Delta\gamma_{ij}$, as defined by Equation (2.15), cannot be accumulated from time step to time step to produce a meaningful definition of strain because the base vectors to which the components of $\Delta\gamma_{ij}$ are referred are redefined for each time step. Thus, $\Delta\gamma_{ij}$ should be interpreted within each time step as a strain increment measured relative to the configuration at the beginning of the time step and referred to the base vectors used in the time step, with the understanding that these increments are not be be accumulated from time step to time step.

The displacement increments Δu_i, on the other hand, can be accumulated from time step to time step to produce the total displacements u_i measured relative to the configuration at the start of the problem. The gradients of the total displacement can be used to compute any desired strain measure. The strain measure that will be used in the constitutive relations is defined in the next section.

3. MATERIAL BEHAVIOR -- CONSTITUTIVE RELATIONS

The theory developed herein is intended to be applicable to materials which exhibit anisotropic elastic-plastic behavior and are subjected to finite deformations. A specific material model is not developed here, but the general nature of the model to be used in the formulation is indicated and the procedure for applying the model is developed.

A prominent characteristic of the general material model assumed in the formulation is time-dependent plastic behavior in which the plastic strain rate depends on stress, a number of history-dependent "internal variables" which characterize the state of the material, and a number of prescribed environmental parameters such as temperature and neutron flux. Several models of this type, based on experimental data, have been proposed, such as the ones by Hart (Reference 3) and Miller (Reference 4).

Another prominent characteristic of the assumed general model is anisotropy of the material. Certain technologically important materials, Zircaloy for example, exhibit anisotropy which is sufficiently significant to require modelling of its effects to achieve an accurate representation of the deformation behavior.

Since anisotropic materials behave differently in different directions, constitutive relations for these materials must be expressed in terms of a definite set of directions or axes, referred to herein as the characteristic axes. In a finite deformation formulation, the effects of rotation of the characteristic axes relative to a fixed frame of reference must be accounted for as the material moves and deforms. In a rigid body motion of the material, the characteristic axes, obviously, remain fixed relative to the material and

rotate relative to the fixed frame of reference with an angular velocity equal to that of the body. An appropriate generalization of this for arbitrary motions is to allow the characteristic axes at each material point to rotate with an angular velocity equal to the spin* at that point. Thus, at a material point, the characteristic axes to which the constitutive relations are referred remain fixed in orientation relative to each other but rotate as a unit as the material moves and deforms.

In formulating constitutive relations, any convenient set of three independent characteristic axes can be used. Most commonly, a set of three mutually orthogonal axes are used since this simplifies the interpretation of stress and strain rate components. Thus, in the formulation discussed below, the characteristic axes are thought of as being mutually orthogonal.**.

The unit base vectors $\bar{e}_I$ of the characteristic axes are defined in terms of the $\bar{G}_i$ and g_i base vectors by the following transformations:

$$\bar{e}_I = Q_I^i \, \bar{G}_i$$

$$= q_I^i \, \bar{g}_i \qquad (3.1a\text{-}c)$$

where $q_I^i \equiv (g_j^i + \Delta u_{;j}^{\,i}) \, Q_I^j$

---

* Spin is a field quality derived from velocity gradients. The spin at a material point can be interpreted as the local angular velocity of the material surrounding the point (Reference 5).

** The mathematical developments are not restricted to the orthogonal case, but the interpretation of the stress and strain rate components will differ from those given here if non-orthogonal characteristic axes are used.

The stress tensor σ^{IJ} and strain rate tensor $\dot{\epsilon}_{IJ}$ used in the constitutive relations are related to τ^{ij} and $\dot{\gamma}_{ij}$ by

$$\tau^{ij} = Q_I^i \sigma^{IJ} Q_J^j$$

$$\dot{\epsilon}_{IJ} = Q_I^i \dot{\gamma}_{ij} Q_J^j \qquad (3.2a,b)$$

σ^{IJ} is the Cauchy stress tensor, with components referred to the (rotating) characteristic axes. These stress components are the so-called true stresses which are interpreted as force per unit of current area. The ordinary time derivative of σ^{IJ} is the stress rate tensor $\dot{\sigma}^{IJ}$ which corresponds to the Jaumann stress rate tensor (Reference 6) with components referred to the characteristic axes.

The strain rate tensor $\dot{\epsilon}_{IJ}$ corresponds to the deformation rate tensor with components referred to the characteristic axes. These strain rate components are the so-called true strain rates which are interpreted as follows: A normal component $\dot{\epsilon}_{IJ}$ (I=J) is the rate of change of length per unit current length of a material line segment instantaneously coinciding with the I characteristic axis. A shear component $\dot{\epsilon}_{IJ}$ ($I \neq J$) is one-half the rate of decrease of the angle between two material line segments instantaneously coinciding with the (orthogonal) I and J characteristic axes, respectively.

The total strain rate is assumed to be composed of a sum of strain rates from different mechanisms, as follows:

$$\dot{\epsilon}_{IJ} = \dot{\epsilon}^e_{IJ} + \dot{\epsilon}^p_{IJ} + \dot{\epsilon}^g_{IJ} \qquad (3.3)$$

where $\dot{\epsilon}^e_{IJ}$ is the elastic strain rate, $\dot{\epsilon}^p_{IJ}$ is the plastic strain rate, and $\dot{\epsilon}^g_{IJ}$ is the stress-independent growth strain rate. The plastic strain rate may, itself, be composed of contributions from different plastic strain mechanisms, such as thermal creep, neutron flux induced creep, and so forth. The growth strain rate may also be composed of contributions from different mechanisms such as thermal expansion and irradiation growth.

The elastic strain rate, in general, depends on stress and stress rate along with the environmental variables, such as temperature. The specific form of the elastic behavior is not of prime importance as far as the mathematical formulation of the solution procedure is concerned. For definiteness, hypoelastic behavior will be assumed here, in which the elastic strain rate is linearly related to stress rate as follows:

$$\dot{\epsilon}^{e}_{IJ} = C^{e}_{IJKL}\, \dot{\sigma}^{KL} \tag{3.4}$$

where C^{e}_{IJKL} is the elastic compliance tensor which may be temperature dependent. The incremental form of this relation, resulting from integration over a time step, can be approximated as follows:

$$\Delta\epsilon^{e}_{IJ} \approx C^{e}_{IJKL}\, \Delta\sigma^{KL} \tag{3.5}$$

where the elastic compliance tensor is understood to be evaluated at the average temperature of the time step.

The plastic strain rate depends on stress, history-dependent "internal variables" which characterize the state of the material, and environmental variables such as temperature and neutron flux. In the incremental solution procedure developed here, it is necessary to obtain an appropriate expression which linearly relates the plastic strain increments to the stress increments. This can be done by first expanding the plastic strain rate in a Taylor series about the known stress state σ^{IJ}_{o} at the beginning of a time step. The linear part of this Taylor series expansion is

$$\dot{\epsilon}^{p}_{IJ} \approx \dot{\epsilon}^{p_o}_{IJ} + \frac{\partial \dot{\epsilon}^{p_o}_{IJ}}{\partial \sigma^{KL}} (\sigma^{KL} - \sigma^{KL}_{o}) \tag{3.6}$$

In the above, expression, $\dot{\epsilon}^{p_o}_{IJ}$ and the partial derivatives are evaluated at constant stress σ^{IJ}_{o}. Now, letting σ^{KL} be the average stress of a time

step (i.e., $\sigma^{KL} = \sigma_o^{KL} + \frac{1}{2} \Delta\sigma^{KL}$) and integrating the above expression over a time step results in

$$\Delta\epsilon_{IJ}^{p} \approx \Delta\epsilon_{IJ}^{p_o} + C_{IJKL}^{p_o} \Delta\sigma^{KL} \tag{3.7}$$

where

$$\Delta\epsilon_{IJ}^{p_o} = \int_{t_o}^{t} \dot{\epsilon}_{IJ}^{p_o} \, dt$$

$$C_{IJKL}^{p_o} = \frac{1}{2} \int_{t_o}^{t} \frac{\partial \dot{\epsilon}_{IJ}^{p_o}}{\partial \sigma^{KL}} \, dt \tag{3.8a,b}$$

In the above, $\Delta\epsilon_{IJ}^{p_o}$ is the plastic strain increment that would occur if the stress was held constant at the value σ_o^{IJ} throughout the time step. $C_{IJKL}^{p_o}$ is called the plastic compliance tensor.

The growth strain rate depends on the environmental variables and not on stress. The increment in growth strain is

$$\Delta\epsilon_{IJ}^{g} = \int_{t_o}^{t} \dot{\epsilon}_{IJ}^{g} \, dt \tag{3.9}$$

The numerical method used to evaluate the integrals in Equations (3.8) and (3.9) will not be specified here, since its design depends on the specific material model used. For some relatively simple models it is possible to evaluate the integrals analytically, for other more complex models it is necessary to evaluate the integrals numerically.

Combining equations (3.3), (3.5), (3.7), and (3.9) results in an approximate incremental constitutive relation in the following form:

$$\Delta\epsilon_{IJ} \approx \Delta\epsilon^{*}_{IJ} + C_{IJKL}\ \Delta\sigma^{KL} \tag{3.10}$$

where

$$\Delta\epsilon^{*}_{IJ} = \Delta\epsilon^{p_o}_{IJ} + \Delta\epsilon^{g}_{IJ} \tag{3.11a}$$

$$C_{IJKL} = C^{e}_{IJKL} + C^{p_o}_{IJKL} \tag{3.11b}$$

The inverse relation is

$$\Delta\sigma^{IJ} \approx D^{IJKL}\ \Delta\epsilon_{KL} - \Delta\sigma^{IJ}_{*} \tag{3.12}$$

where D^{IJKL}, the stiffness tensor, is the inverse of C_{IJKL}, and

$$\Delta\sigma^{IJ}_{*} = D^{IJKL}\ \Delta\epsilon^{*}_{KL} \tag{3.13}$$

The stress and strain increments appearing in the above incremental constitutive relations have components referred to the rotating characteristic axes. In order to apply these constitutive relations in an incremental solution procedure, it is necessary to derive a procedure for keeping track of the rotating characteristic axes and to derive expressions which relate $\Delta\gamma_{ij}$ to $\Delta\epsilon_{IJ}$ and $\Delta\gamma_{ij}$ to $\Delta\tau^{ij}$.

To derive the procedure for keeping track of the rotating characteristic axes, it is recalled that the $\bar{e}_I$ base vectors do not change in magnitude but they rotate with an angular velocity $\bar{\omega}$, given by Equation (2.16). Therefore, the time derivative of $\bar{e}_I$ is

$$\dot{\bar{e}}_I = \bar{\omega} \times \bar{e}_I \tag{3.14}$$

which, along with Equation (3.1a) results in

$$\dot{Q}^{i}_{I}\ \bar{G}_i + Q^{i}_{I}\ \dot{\bar{G}}_i = Q^{i}_{I}\ (\bar{\omega} \times \bar{G}_i) \tag{3.15}$$

Taking the dot product of both sides of the above equation with $\bar{G}_j$ gives an equation which, when simplified, results in

$$\dot{Q}^{i}_{I}\ G_{ij} + \tfrac{1}{2}\ Q^{i}_{I}\ \dot{G}_{ij} = 0 \tag{3.16}$$

This equation can be written in matrix form as

$$[G][\dot{Q}] + \tfrac{1}{2}\,[\dot{G}][Q] = 0 \tag{3.17}$$

the solution of which is

$$[G]^{\frac{1}{2}}[Q] = \text{constant} = [G_o]^{\frac{1}{2}}[Q_o] = [Q_o]$$

$$[Q] = [G]^{-\frac{1}{2}}[Q_o] \tag{3.18}$$

where $[G]^{\frac{1}{2}}$, the "square root" of $[G]$, is the 3x3 symmetric matrix such that

$$[G] = [G]^{\frac{1}{2}}[G]^{\frac{1}{2}} \tag{3.19}$$

$[G]^{\frac{1}{2}}$ can be computed by finding the eigenvalues and eigenvectors of $[G]$; i.e., by finding the orthogonal matrix $[\varphi]$ and the diagonal matrix $[\lambda]$ whose diagonal elements are the eigenvalues, such that

$$[\varphi]^T[G][\varphi] = [\lambda]$$

$$[\varphi][\lambda][\varphi]^T = [G] \tag{3.20a-c}$$

$$[\varphi]^T[\varphi] = [I]$$

Then

$$[G]^{\frac{1}{2}} = [\varphi][\lambda]^{\frac{1}{2}}[\varphi]^T \tag{3.21a,b}$$

$$[G]^{-\frac{1}{2}} = [\varphi][\lambda]^{-\frac{1}{2}}[\varphi]^T$$

where $[\lambda]^{\frac{1}{2}}$ is the diagonal matrix whose diagonal elements are the square roots of the corresponding elements of $[\lambda]$.

$[G]^{-\frac{1}{2}}$ can also be computed from the following series expansion:

$$[G]^{-\frac{1}{2}} = [[I] + [\Delta G]]^{-\frac{1}{2}}$$

$$= [[I] + 2\,[\Delta\gamma]]^{-\frac{1}{2}}$$

$$= [I] - [\Delta\gamma] + \frac{3}{2!}[\Delta\gamma]^2 - \frac{3\times5}{3!}[\Delta\gamma]^3 + \frac{3\times5\times7}{4!}[\Delta\gamma]^4 - \ldots \tag{3.22}$$

To derive the expression relating $\Delta\gamma_{ij}$ to $\Delta\epsilon_{IJ}$, it is noted that by using Equation (3.18), Equation (3.2b) can be written in matrix form as

$$\begin{aligned}[\dot{\epsilon}] &= [Q]^T[\dot{\gamma}][Q] \\ &= \tfrac{1}{2}[Q]^T[\dot{G}][Q] \\ &= \tfrac{1}{2}[Q_o]^T[G]^{-\frac{1}{2}}[\dot{G}][G]^{-\frac{1}{2}}[Q_o] \end{aligned} \tag{3.23}$$

The above equation can be integrated to give

$$[\Delta\epsilon] = \tfrac{1}{2}[Q_o]^T(\ln[G])[Q_o] \tag{3.24}$$

where the natural log of $[G]$ is defined by

$$(\ln[G]) = [\varphi](\ln[\lambda])[\varphi]^T \tag{3.25}$$

and $(\ln[\lambda])$ is the diagonal matrix whose diagonal elements are the natural logs of the corresponding elements of $[\lambda]$.

$(\ln[G])$ can also be computed from the following series expansion

$$\begin{aligned}(\ln[C]) &= (\ln[[I] + [\Delta G]]) \\ &= (\ln[[I] + 2[\Delta\gamma]]) \\ &= 2[\Delta\gamma] - \frac{2^2}{2}[\Delta\gamma]^2 + \frac{2^3}{3}[\Delta\gamma]^3 - \ldots \end{aligned} \tag{3.26}$$

By using Equations (3.2), (3.12), (3.18), (3.22), (3.24), and (3.26), and neglecting second order terms involving $\Delta\gamma_{ij}$, the following approximate expression relating $\Delta\gamma_{ij}$ to $\Delta\tau^{ij}$ can be derived:

$$\Delta\tau^{ij} \approx [D^{ijkl} - \tfrac{1}{2}(\tau_*^{il}g^{jk} + \tau_*^{lj}g^{ik} + \tau_*^{ik}g^{jl} + \tau_*^{kj}g^{il})]\Delta\gamma_{kl} - \Delta\tau_*^{ij} \tag{3.27}$$

where

$$\begin{aligned}\tau_*^{ij} &= \tau_o^{ij} - \Delta\tau_*^{ij} \\ \Delta\tau_*^{ij} &= Q_{o_I}^{\ i}\,\Delta\sigma_*^{IJ}\,Q_{oJ}^{\ j} \\ D^{ijkl} &= Q_{o_I}^{\ i}\,Q_{o_J}^{\ j}\,D^{IJKL}\,Q_{o_K}^{\ k}\,Q_{o_L}^{\ l} \end{aligned} \tag{3.28a-c}$$

By combining the terms in square brackets and denoting the result by D_*^{ijkl}, Equation (3.27) can be written as

$$\Delta\tau^{ij} \approx D_*^{ijkl}\ \Delta\gamma_{kl} - \Delta\tau_*^{ij} \tag{3.29}$$

where

$$D_*^{ijkl} = D^{ijkl} - \tfrac{1}{2}(\tau_*^{il} g^{jk} + \tau_*^{lj} g^{ik} + \tau_*^{ik} g^{jl} + \tau_*^{kj} g^{il}) \tag{3.30}$$

4. VIRTUAL WORK EQUATION

Let $\delta\bar{v}$ denote an arbitrary virtual change or variation of the velocity field such that the appropriate components of $\delta\bar{v}$ vanish on the part of the surface where displacements are prescribed.

$$\delta\bar{v} = \delta v^i \bar{g}_i = \delta v_i \bar{g}^i \qquad (4.1a,b)$$

The corresponding variation of the strain rate field is

$$\delta\dot{\gamma}_{mn} = \tfrac{1}{2}[(g^i_m + \Delta u^i_{;m})\delta v_{i;n} + (g^i_n + \Delta u^i_{;n})\delta v_{i;m}] \qquad (4.2)$$

The Principle of Virtual Work, which is a statement of equilibrium, is expressed by the following virtual work equation:

$$\int_V \tau^{mn}\delta\dot{\gamma}_{mn}dV - \int_S \bar{T}\cdot\delta\bar{v}dS - \int_V \rho\bar{\bar{F}}\cdot\delta\bar{v}dV = 0 \qquad (4.3)$$

The integrals in this equation are evaluated at time t.

In order to apply the virtual work equation to formulate the finite element equilibrium equation, it is necessary to transform the integrals so they can be evaluated in the known configuration of the body at time t_o. The volume integrals can be transformed by using the volume transformation relations given by Equation (2.18), which, along with Equation (4.2) allows the internal virtual work term to be written as

$$\int \tau^{mn}\delta\dot{\gamma}_{mn}dV = \int_{V_o} J\tau^{mn}\delta\dot{\gamma}_{mn}dV_o$$

$$= \int_{V_o} J\tau^{mn}(g^i_m + \Delta u^i_{;m})\delta v_{i;n}dV_o \qquad (4.4)$$

The body force term can be written as

$$\int_V \rho \bar{F}.\delta\bar{v}dV = \int_{V_o} \rho_o \bar{F}.\bar{g}^i \delta v_i dV_o$$

$$= \int_{V_o} \rho_o f^i \delta v_i dV_o \tag{4.5}$$

The treatment of the surface traction term depends on the nature of the prescribed surface traction. For a pressure load, the most common type of surface traction, the traction vector is of the form

$$\bar{T} = -p\bar{N}$$

$$= -pN_k \bar{G}^k \tag{4.6}$$

where p is the pressure and $\bar{N}$ is the unit vector normal to the surface. Letting S_p denote the part of the surface over which pressure loads are prescribed, the contribution from S_p to the surface traction term becomes

$$\int_{S_p} \bar{T}.\delta\bar{v}dS = -\int_{S_p} p\bar{N}.\delta\bar{v}dS$$

$$= -\int_{S_p} pN_k(\bar{G}^k.\bar{g}_i)\delta v^i dS$$

$$= -\int_{S_p^o} pn_k \quad J\ (\bar{G}^k.\bar{g}_i)\delta v^i dS_o \tag{4.7}$$

where the surface transformation relation given by Equation (2.20) has been used. A representation of $J(\bar{G}^k.\bar{g}_i)$ in terms of displacement gradients can be derived as follows:

$$J\ (\bar{G}^k.\bar{g}_i) = \tfrac{1}{2}e^{kmn}(\bar{G}_m x \bar{G}_n).\bar{g}_i/\sqrt{g}$$

$$= \tfrac{1}{2}e^{kmn}(g_m^r + \Delta u_{;m}^r)(g_n^s + \Delta u_{;n}^s)(\bar{g}_r x \bar{g}_s).\bar{g}_i/\sqrt{g}$$

$$= \tfrac{1}{2}e^{kmn}e_{rsi}(g_m^r + \Delta u_{;m}^r)(g_n^s + \Delta u_{;n}^s)$$

$$= g_i^k\ (1 + \Delta u_{;j}^j) - \Delta u_{;i}^k + \tfrac{1}{2}e^{kmn}e_{rsi}\Delta u_{;m}^r \Delta u_{;n}^s \tag{4.8}$$

Therefore, Equation (4.7) can be written as

$$\int_{S_p} \bar{T}.\delta\bar{v}dS = -\int_{S_p^o} p[n_i + n_k (g_i^k \Delta u^j_{;j} - \Delta u^k_{;i} + \tfrac{1}{2} e^{kmn} e_{rsi} \Delta u^r_{;m} \Delta u^s_{;n})]\delta v^i dS_o \qquad (4.9)$$

Substituting Equations (4.4), (4.5), and (4.9) into (4.3) results in the following virtual work equation for the case when the prescribed tractions are pressure loads:

$$\int_{V_o} J\tau^{mn}(g^i_m + \Delta u^i_{;m})\delta v_{i;n} dV_o - \int_{V_o} \rho_o f^i \delta v_i dV_o$$

$$+\int_{S_p^o} p[n_i + n_k(g_i^k \Delta u^j_{;j} - \Delta u^k_{;i} + \tfrac{1}{2} e^{kmn} e_{rsi} \Delta u^r_{;m} \Delta u^s_{;n})]\delta v^i dS_o = 0 \qquad (4.10)$$

By substituting Equations (2.15), (2.19), (3.28), and (3.29) into the above and neglecting all second and higher order terms involving the displacement gradient increments, the following approximate form of the virtual work equation can be derived:

$$\left\{ \int_{V_o} (D_*^{injk} + \tau_*^{kn} g^{ij} + \tau_*^{in} g^{jk}) \Delta u_{j;k} \delta v_{i;n} dV_o \right.$$

$$\left. + \int_{S_p^o} p(n^i g^{jk} - n^j g^{ik}) \Delta u_{j;k} \delta v_i dS_o \right\}$$

$$- \left\{ \int_{V_o} \rho_o \Delta f^i \delta v_i dV_o + \int_{V_o} \Delta\tau_*^{in} \delta v_{i;n} dV_o - \int_{S_p^o} \Delta p n^i \delta v_i dS_o \right\}$$

$$+ \left\{ \int_{V_o} \tau_o^{mn} \delta v_{m;n} dV_o - \int_{V_o} \rho_o f_o^i \delta v_i dV_o + \int_{S_p^o} p_o n^i \delta v_i dS_o \right\} \approx 0 \qquad (4.11)$$

The following relations involving the body force and pressure were used in deriving the above equation:

$$f^i = f_o^i + \Delta f^i \qquad (4.12a,b)$$

$$p = p_o + \Delta p$$

5. FINITE ELEMENT EQUILIBRIUM EQUATION

The virtual work equation derived in the previous section forms the foundation from which the finite element equilibrium equation is derived. A three-dimensional isoparametric finite element formulation will be used here, in which the coordinates at time t_o and t, the displacement increments, and the displacement gradient increments are approximated as follows:

$$x_j \approx N^\beta x_{j\beta}$$

$$X_j = x_j + \Delta u_j \approx N^\beta (x_{j\beta} + \Delta u_{j\beta}) = N^\beta X_{j\beta}$$

$$\Delta u_j \approx N^\beta \Delta u_{j\beta} \qquad (5.1a\text{-}d)$$

$$\Delta u_{j;k} \approx N^\beta_{;k} \Delta u_{j\beta}$$

where $x_{j\beta}$ and $\Delta u_{j\beta}$ are the coordinates and displacement increments at node β of the element and N^β is the isoparametric shape function which assumes a unit value at node β and a zero value at all other nodes of the element.

Likewise, the velocity variations and their gradients are approximated by

$$\delta v_i \approx N^\alpha \delta v_{i\alpha} \qquad (5.2a,b)$$

$$\delta v_{i;n} \approx N^\alpha_{;n} \delta v_{i\alpha}$$

Substitution of Equations (5.1) and (5.2) into Equation (4.11) results in the finite element form of the approximate virtual work equation. This equation, after elimination of the arbitrary $\delta v_{j\beta}$ from all terms, becomes the following approximate finite element equilibrium equation:

$$K^{i\alpha j\beta} \Delta u_{j\beta} \approx \Delta f^{i\alpha} - f_R^{i\alpha} \qquad (5.3)$$

The terms appearing in this equation are defined and discussed below:

$\Delta f^{i\alpha}$ is the increment in nodal force which contains contributions from different sources, as follows:

$$\Delta f^{i\alpha} = \Delta f_p^{i\alpha} + \Delta f_B^{i\alpha} + \Delta f_*^{i\alpha} \tag{5.4}$$

where

$$\Delta f_p^{i\alpha} = -\int_{S_p^o} \Delta p n^i N^\alpha dS_o$$

$$\Delta f_B^{i\alpha} = \int_{V_o} \rho_o \Delta f^i N^\alpha dV_o \tag{5.5a-c}$$

$$\Delta f_*^{i\alpha} = \int_{V_o} \Delta \tau_*^{in} N^\alpha_{;n} dV_o$$

In the above, $\Delta f_p^{i\alpha}$ is the increment in nodal force due to pressure increments, $\Delta f_B^{i\alpha}$ is due to body force increments, and $\Delta f_*^{i\alpha}$ is due to plastic and growth strain increments.

$f_R^{i\alpha}$ in Equation (5.3) is the residual or unequilibrated nodal force defined by

$$f_R^{i\alpha} = \int_{V_o} \tau_o^{in} N^\alpha_{;n} dV_o - \int_{V_o} \rho_o f_o^i N^\alpha dV_o + \int_{S_p^o} p_o n^i N^\alpha dS_o \tag{5.6}$$

The residual force results from the last group of terms enclosed by braces in Equation (4.11). This group of terms is actually the virtual work equation for the solution state at the beginning of the time step. Therefore, if the stress state τ_o^{ij} was in equilibrium with the prescribed body force f_o^i and surface pressure p_o, the sum of these terms would be zero. However, since second order terms were neglected in developing Equation (4.11), this equation is not an exact statement of equilibrium, which results in a computed solution which does not exactly satisfy equilibrium. The negative of the residual nodal force, as it appears in Equation (5.3), is the nodal force which would be required to cause the stress state τ_o^{ij} to change into one which is, in the finite element

sense, in equilibrium with the applied loads. The residual force term, then, acts as a correction which tends to increase the numerical stability and accuracy of the approximate solution process. The technique of using residual force correction was apparently first reported in the open literature by Hofmeister, Greenbaum, and Evensen in Reference (7).

The "stiffness matrix" $K^{i\alpha j\beta}$ in Equation (5.3) can be decomposed into the sum of several contributions, as follows:

$$K^{i\alpha j\beta} = K_1^{i\alpha j\beta} + K_2^{i\alpha j\beta} + K_3^{i\alpha j\beta} + K_4^{i\alpha j\beta} + K_5^{i\alpha j\beta} \tag{5.7}$$

where

$$K_1^{i\alpha j\beta} = \int_{V_o} D^{injk} N^{\alpha}_{;n} N^{\beta}_{;k} dV_o$$

$$K_2^{i\alpha j\beta} = \int_{V_o} -\tfrac{1}{2}(\tau_*^{kn} g^{ij} + \tau_*^{ij} g^{kn} + \tau_*^{ik} g^{nj} + \tau_*^{nj} g^{ik}) N^{\alpha}_{;n} N^{\beta}_{;k} dV_o$$

$$K_1^{i\alpha j\beta} + K_2^{i\alpha j\beta} = \int_{V_o} D_*^{injk} N^{\alpha}_{;n} N^{\beta}_{;k} dV_o \tag{5.8a-g}$$

$$K_3^{i\alpha j\beta} = \int_{V_o} \tau_*^{kn} g^{ij} N^{\alpha}_{;n} N^{\beta}_{;k} dV_o$$

$$K_2^{i\alpha j\beta} + K_3^{i\alpha j\beta} = \int_{V_o} \tfrac{1}{2}(\tau_*^{kn} g^{ij} - \tau_*^{ij} g^{kn} - \tau_*^{ik} g^{nj} - \tau_*^{nj} g^{ik}) N^{\alpha}_{;n} N^{\beta}_{;k} dV_o$$

$$K_4^{i\alpha j\beta} = \int_{V_o} \tau_*^{in} g^{jk} N^{\alpha}_{;n} N^{\beta}_{;k} dV_o$$

$$K_5^{i\alpha j\beta} = \int_{S_p^o} p(n^i g^{jk} - n^j g^{ik}) N^{\alpha} N^{\beta}_{;k} dS_o$$

The K_1 contribution to the stiffness matrix corresponds to the usual stiffness matrix which results from an infinitesimal deformation formulation. The K_2 through K_5 contributions, which do not appear in an infinitesimal deformation formulation, are the result of taking finite deformations into account.

The $K_1 + K_2$ contribution is identical in form to the K_1 contribution; i.e., it can be computed in the same way as K_1 by using D_* in place of D.

Contributions similar to K_2, K_3, and K_4 have been identified previously by other authors who call various combinations of these terms the "initial stress stiffness matrix." The difference between the present and previous formulations is that $\tau_*^{ij} = \tau_o^{ij} - \Delta\tau_*^{ij}$ appears in the present formulation where τ_o^{ij} appears in previous formulations. It is necessary to include the $\Delta\tau_*^{ij}$ term if thermal or irradiation growth strain increments are present or if an estimate of the plastic strain increment is available as it is in the present formulation. The initial stress contributions to the stiffness matrix were apparently first defined unambiguously by Martin in Reference 8 and used in an elastic-plastic formulation by Hibbitt, Marcal, and Rice in Reference 9.

The K_4 contribution can be associated with volume change which takes place during the time step. K_4 would not be present if the approximation $J \approx 1$ had been used during the time step instead of $J \approx 1 + \Delta u^i_{;i}$. Also, K_4 would not be present if the volume change term was imbedded in the definition of stress used in the constitutive relations. That is, if a stress tensor S^{IJ} had been used in the constitutive relations instead of σ^{IJ}, where $S^{IJ} = \frac{\rho_{ref}}{\rho}\ \sigma^{IJ}$, with ρ being the density in the current configuration and ρ_{ref} being the density in a reference configuration.

The K_5 contribution accounts for the change in area and orientation of the surface over which pressure is applied. This contribution was apparently first defined explicitly in Reference 9 by Hibbitt, Marcal, and Rice, who call it the "initial load stiffness matrix."

The K_1 through K_3 contributions satisfy symmetry relations of the form $K^{i\alpha j\beta} = K^{j\beta i\alpha}$. K_4 and K_5, however, do not satisfy these symmetry relations. Therefore, an unsymmetric equation solver is necessary if K_4 and K_5 are included in the formulation. The solution of unsymmetric equations requires more computer time and storage over that required by symmetric equations, which leads to the conjecture that it may be more efficient to neglect the K_4 and K_5 contributions (along with the second order terms already neglected), use smaller time steps, and rely on the residual force to correct the errors caused by the neglected terms. This approach, where K_4 and K_5 are neglected, has been taken in the ACCEPT program (Reference 1), where the theory developed herein has been implemented.

6. INCREMENTAL SOLUTION PROCEDURE AND TIME STEP CONTROL

The equations which govern the increments in stress, strain, and displacement which occur during a time step were derived in the preceding sections. The procedure for implementing these equations in a computer program is summarized in this section and a time step control algorithm is given for computing appropriate time step sizes, based on the progress of the solution. The time step control algorithm presumes that the very first time step size is prescribed and, upon completion of any time step, determines whether the time step size is acceptable (sufficiently small) and determines the time step size to be used in the next time step.

The first major task which must be performed at the beginning of a time step is to compute the finite element stiffness matrix and nodal force vector for each element. To accomplish this for a particular element, calculations involving the constitutive equations must be performed at each integration or Gauss point of the element. This involves first calculating $\Delta\epsilon^{*}_{IJ}$ and C_{IJKL} of Equation (3.10), then calculating $\Delta\sigma^{IJ}_{*}$ and D^{IJKL} of Equation (3.12), and finally calculating $\Delta\tau^{ij}_{*}$, τ^{ij}_{*}, and D^{ijkl}_{*} of Equations (3.28) and (3.29). The element stiffness matrix and force vectors of Equation (5.3) are then computed, using Equations (5.4) - (5.8). It should be noted that the calculated quantities $\Delta\sigma^{IJ}_{*}$ and D^{IJKL} appearing in Equation (3.12) can be saved for use later on in calculating stress increments, to avoid the necessity of re-evaluating these quantities.

The next major task is to solve the finite element equilibrium or stiffness equations for the nodal displacement increments. This is accomplished by using the bandwidth, wavefront, or iterative equation

solver available in any general-purpose finite element program.

Having calculated the nodal displacement increments, the next major task is to calculate increments in the various field quantities, consistent with the calculated displacement increments. This is accomplished by following the sequence of calculations described below for each integration or Gauss point of each finite element:

1. Calculate the displacement gradient increments $\Delta u_{i;j}$ using Equation (5.1d).

2. Calculate the metric tensor G_{ij} using Equations (2.4) and (2.13). Calculate the eigenvalues and eigenvectors of G_{ij}. (See Equation (3.20)).

3. Calculate Q_I^i using Equations (3.18) and (3.21b). Calculate q_I^i using Equation (3.1c). Note that q_I^i corresponds to the initial value of the transformation matrix Q_I^i for the next time step because the $\bar{G}_i$ base vectors are always redefined to coincide with the $\bar{g}_i$ base vectors at the beginning of a time step.

4. Calculate the strain increments $\Delta\epsilon_{IJ}$ using Equations (3.24) and (3.25).

5. Calculate the stress increments $\Delta\sigma^{IJ}$ by applying two iterations of the Newton-Raphson method to solve the following nonlinear equation for $\Delta\sigma^{IJ}$:

$$\Delta\epsilon_{IJ} = \Delta\epsilon_{IJ}^{e} + \Delta\epsilon_{IJ}^{pa} + \Delta\epsilon_{IJ}^{g} \tag{6.1}$$

where $\Delta\epsilon_{IJ}^{pa}$ is the plastic strain increment evaluated at the average stress $\sigma_a{}^{IJ} = \sigma_o{}^{IJ} + \frac{1}{2}\Delta\sigma^{IJ}$ of the time step.

The stress increment $\Delta\sigma_1{}^{IJ}$ of the first iteration is calculated using Equation (3.12) and the stress increment $\Delta\sigma^{IJ}$ of the second iteration is calculated by solving the following linear equation:

$$\Delta\epsilon_{IJ} \approx \Delta\epsilon^{pl}_{IJ} + \Delta\epsilon^{g}_{IJ} - C^{pl}_{IJKL}\Delta\sigma_1{}^{KL} + (C^{e}_{IJKL} + C^{pl}_{IJKL})\Delta\sigma^{KL} \tag{6.2}$$

where $\Delta\epsilon^{pl}_{IJ}$ and C^{pl}_{IJKL} are evaluated at the stress $\sigma_1{}^{IJ} = \sigma^{IJ}_o + \frac{1}{2}\Delta\sigma_1{}^{IJ}$.

The stress increment $\Delta\sigma^{IJ}$ resulting from the second iteration is taken to be the stress increment of the time step. In order for this to be an accurate approximation, it is necessary to require the "stress error" σ^{IJ}_{err} defined by

$$\sigma^{IJ}_{err} = \Delta\sigma^{IJ} - \Delta\sigma^{IJ}_1 \tag{6.3}$$

to be sufficiently small. This requirement is enforced by the time step control algorithm described below.

The next major task is to determine whether the time step size used in the current time step is sufficiently small and to determine the time step size to be used in the next time step. The four basic points discussed below must be considered in making these determinations.

1. All second and higher order terms involving displacement gradient increments were neglected to develop the approximate virtual work equation. In order for this to be an accurate approximation, it is necessary to require the displacement gradient increments to be sufficiently small.

2. The approximate incremental constitutive relation of Equation (3.10) was also used to develop the approximate virtual work equation. In order for this to be an accurate approximation, it is necessary to require the stress error defined by Equation (6.3) to be sufficiently small. Also, it is necessary to limit the size of the temperature increment if the elastic compliance is temperature-dependent (see Equation (3.5)), or if an average-temperature approximation is used in evaluating the integrals of Equation (3.8).

3. The total compliance tensor as defined in Equation (3.11b) is composed of an elastic compliance C^{e}_{IJKL} and a plastic compliance C^{po}_{IJKL}, the latter of which increases monotonically as the time step size increases. C^{po}_{IJKL} is singular (does not possess an inverse) if the material is, as usually assumed, plastically-incompressible. If the time step size is sufficiently large to cause the plastic compliance to be large relative to the elastic compliance, then the total compliance tensor will be nearly singular. Since a nearly singular compliance leads to an ill-conditioned set of finite element equilibrium equations which is difficult to solve accurately, it is necessary to limit the time step size such that the plastic compliance is not too large compared to the elastic compliance.

4. The finite element stiffness matrix contains contributions due to the stress quantity $\tau^{ij}_{*} = \tau^{ij}_{o} - \Delta\tau^{ij}_{*}$. The quantity $\Delta\tau^{ij}_{*}$ depends on the plastic and growth strain increments as defined by Equations (3.11a), (3.13), and (3.28b). If the contributions to the stiffness matrix due to $\Delta\tau^{ij}_{*}$ are allowed to be too large, this, like a nearly-singular compliance tensor, can lead to an ill-conditioned set of finite element equations. Therefore, it is necessary to limit the magnitude of the $\Delta\tau^{ij}_{*}$ contributions. This can be accomplished in effect by limiting the plastic strain increments and the temperature increments.

The four major points discussed above are accounted for in the time step control algorithm described below. The following definitions are necessary in order to completely describe the algorithm:

DGA = Prescribed maximum allowable displacement gradient increment. (Recommended to be in the range 0.001 to 0.05.)

DGD = Prescribed maximum desired displacement gradient increment. (Recommended to be approximately equal to DGA/5, but not larger than DGA/2).

DGM = Actual maximum displacement gradient increment occurring during the current time step.

ETA, ETD, ETM = Same as above but for total strain increments.

EPA, EPD, EPM = Same as above but for plastic strain increments.

SEA, SED, SEM = Same as above but for "stress errors" as defined in Equation (6.3). (SEA recommended to be 1 to 5 percent of the expected maximum stress.)

CRD = Prescribed maximum desired ratio of plastic compliance to elastic compliance. (Recommended to be 10 to 20.)

CRM = Maximum ratio of plastic compliance to elastic compliance computed during the current time step. The plastic compliance is defined in this sense to be $\int_{t_0}^{t} \frac{\partial \dot{\epsilon}^P}{\partial \sigma} dt$, where $\dot{\epsilon}^P$ and σ are generalized plastic strain rate and stress measures. The elastic compliance is defined to be 1./E, where E is a representative elastic modulus of the material.

The first task performed by the time step control algorithm is to decide whether or not the time step size Δt_{old} of the current time step is sufficiently small. This decision is based on whether or not the following inequalities are satisfied:

$$DGM \leq DGA$$

$$ETM \leq ETA$$

$$EPM \leq EPA$$

$$SEM \leq SEA$$

If any of the inequalities is not satisfied, Δt_{old} is too large and the time step must be redone using a new time step size $\Delta t_{new} < \Delta t_{old}$, as determined below. If all of the inequalities are satisfied, Δt_{old} is sufficiently small and it is permissible to go on to the next time step, using the time step size Δt_{new} determined below.

The next task performed by the time step control algorithm is to choose the new time step size. The algorithm chooses Δt_{new} to be the smallest of a number of candidates Δt_i which are defined as follows:

$\Delta t_1 = (DGD/DGM)\Delta t_{old}$

$\Delta t_2 = (ETD/ETM)\Delta t_{old}$

$\Delta t_3 = (EPD/EPM)\Delta t_{old}$

$\Delta t_4 = (SED/SEM)^{\frac{1}{2}}\Delta t_{old}$ (See footnote 1)

$\Delta t_5 = (CRD/CRM)\Delta t_{old}$

Δt_6 = time step size which would result in a temperature increment not exceeding a prescribed allowable value.

$\Delta t_7 = (M)\Delta t_{old}$, where M is a prescribed number recommended to be in the range 2 to 10.

Δt_8 = prescribed maximum allowable time step size.

---

1. The square root of SED/SEM is used because the "stress error" is approximately proportional to Δt^2.

If the current time step is determined to be acceptable, it is necessary, before beginning the next time step, to update the values of the "essential variables" which are needed to perform each time step. The essential variables are the nodal coordinates $X_{i\alpha}$, and the integration or Gauss point stresses σ^{IJ}, transformation matrices Q_I^i, and any internal variables used in the material model. Also, any other variables which are desired to be output from the program (such as total displacements, total strains, plastic strains, etc.) must be kept track of and updated before each time step.

7. CONCLUSIONS

A finite element procedure has been developed for finite deformation analysis of continuum structures with time-dependent anisotropic elastic-plastic material behavior. The kinematics of deformation are described by using an updated Lagrangian formulation in which the configuration at the beginning of each time step serves as the Lagrangian frame of reference for that time step. The time-history of the solution is generated by using a linear incremental procedure with residual force correction and automatic time step control.

As part of the overall procedure, a sub-procedure has been developed for keeping track, at each material point, of a set of three mutually orthogonal axes which rotate with the material with an angular velocity equal to the spin rate at the material point. These orthogonal rotating axes are associated with characteristic directions in the material and serve as the frame of reference to which the anisotropic constitutive relations are referred.

Another important part of the overall procedure is an automatic time step control algorithm which monitors the progress of the solution and chooses time step sizes to control the accuracy and numerical stability of the solution. This time step control algorithm is an essential part of the procedure, because it is virtually impossible for an analyst to make a good a priori choice of time step sizes without having a good a priori knowledge of the solution.

The analysis procedure described in this document has been implemented in the ACCEPT computer program described in Reference 1. The effectiveness of the procedure has been demonstrated by extensive numerical experimentation with and production usage of the ACCEPT program. Experience in using ACCEPT has shown that the procedure makes the solution of finite deformation elastic-plastic problems almost as routine as the solution of infinitesimal deformation linear elastic problems.

ACKNOWLEDGEMENTS

The author wishes to thank J. L. Hite for typing the manuscript and R. A. Frederickson, E. Friedman, J. L. Gordon, J. B. Newman, P. L. Pfennigwerth, R. B. Stout, and E. A. Zanoni for reviewing the manuscript.

REFERENCES

1. D. N. Hutula and B. E. Wiancko, "ACCEPT: A Three-Dimensional Finite Element Program for Large Deformation Elastic-Plastic -Creep Analysis of Pressurized Tubes," WAPD-TM-1383, March 1980.

2. A. E. Green and W. Zerna, "Theoretical Elasticity," Oxford University Press, London, Second Edition, 1968.

3. E. W. Hart, "Constitutive Relations for the Nonelastic Deformation of Metals," Transactions of the ASME, Journal of Engineering Materials and Technology, Vol. 98, July 1976, pp 193-202.

4. A. K. Miller, "Predictions of Localized Plastic Flow Conditions in Irradiated Zircaloy Using a Unified Phenomenological Model," Proceedings of the Fourth International Conference on Structural Mechanics in Reactor Technology, Vol. C, Paper C3/8, 1977.

5. C. Truesdell and R. Toupin, "The Classical Field Theories," Section 86, Encyclopedia of Physics, Volume III/1, Springer-Verlag, 1960.

6. Y. C. Fung, "Foundations of Solid Mechanics," Prentice-Hall, 1965, p. 448.

7. L. D. Hofmeister, G. A. Greenbaum, and D. A. Evensen, "Large Strain Elasto-Plastic Finite Element Analysis," AIAA Journal, Volume 9, 1971, pp 1248-1254.

8. H. C. Martin, "Derivation of Stiffness Matrices for the Analysis of Large Deflection and Stability Problems," Proceedings of the First Conference on Matrix Methods in Structural Mechanics, AFFDL-TR-66-80, 1966, pp 697-716.

9. H. D. Hibbitt, P. V. Marcal, and J. R. Rice, "A Finite Element Formulation for Problems of Large Strain and Large Displacement," International Journal of Solids and Structures, Volume 6, 1970, pp 1069-1086.

*U.S. GOVERNMENT PRINTING OFFICE: 1980/603-113/604