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FORMULATION OF GENERAL DISCRETE MODELS OF THERMOMECHANICAL BEHAVIOR OF MATERIALS WITH MEMORY

J. T. ODEN* and G. AGUIRRE RAMIREZ†

University of Alabama in Huntsville

Abstract—This paper is concerned with the development of general discrete models capable of depicting quite general thermomechanical behavior of a broad class of nonlinear materials with memory. Generalizations of the finite-element concept are used in conjunction with Coleman's thermodynamics of simple materials to obtain equations of motion and heat conduction for finite elements of nonlinear continua. The kinematics of finite elements is developed in general terms, with particular emphasis given to the idea that locally homogeneous deformations and temperature fields are equivalent to simplex approximations over an element. Certain basic equations of Coleman's thermodynamical theory of materials are reviewed and used to develop equations governing the behavior of a typical finite element, no restrictions being placed on the order of magnitude of the deformation gradients or temperature gradients. Topological properties of a collection of such elements are introduced to construct consistent discrete models of dissipative media with arbitrary geometry, and initial and boundary conditions.

1. INTRODUCTION

THE formulation of discrete models capable of depicting complicated behavior of certain mechanical systems, dates back to the analytical mechanics of Lagrange. The early efforts, as well as those of the intervening years, had as their objective the development of simplified representations of various phenomena for the purpose of obtaining quantitative information on specific types of mechanical behavior. The well-known method of Rayleigh, introduced in 1877 and generalized by Ritz in 1909, provided a powerful technique for the approximate analysis of continuous bodies. More recently, Biot [1–3] presented variational principles and "Lagrange-type" equations for the analysis of problems in classical linear thermoelasticity and in linear irreversible thermodynamics.

In recent times, two distinct developments have occurred which make possible, for the first time, the rational formulation of general discrete models of nonlinear, dissipative continua. First, there was the development of the concept of finite elements, based on primitive ideas of piecewise approximation, introduced formally in 1956 in connection with the approximate analysis of linear plane elasticity problems [4], and recently expanded and generalized so as to apply to continuous fields in general [5–7]. Second, there was Coleman's development of a general thermodynamics of simple materials [8] which served to generalize or to make obsolete many of the previously held notions on irreversible thermodynamics.

In the present paper, these two developments are brought together and used to obtain general discrete models of thermomechanically simple materials with memory. Significantly,

* Professor of Engineering Mechanics, Research Institute.
† Assistant Professor of Engineering Mechanics.

these models are formulated in a manner consistent with fundamental principles of continuum mechanics, without resorting to special variational principles. Rather, general virtual work expressions are derived for thermomechanically simple media and are used to describe the behavior of finite elements of such media. Since our purpose is to develop a general and consistent theory for developing discrete models of thermomechanical phenomena, we adopt the formalism of direct tensor notation so as to cast the governing equations in invariant forms valid for any choice of coordinate system. The resulting equations apply to an extremely broad class of materials and no restrictions on magnitudes of the deformation gradients, the geometry of the continuum, boundary conditions, isotropy of the media, etc. are introduced. Previous discrete formulations, including those pertaining to perfectly elastic solids, viscous fluids, and equations complementary to Biot's formulation for linear irreversible thermodynamics, can be obtained as special cases of the general formulation presented herein.

Following this introductory section, we review, for completeness, certain aspects of the finite element concept as presented by Oden [7], and lay down general formulae for the construction of finite element models of continuous fields defined on spaces of finite dimension. Here the notion of conjugate fields is re-examined as a natural vehicle for obtaining "generalized variables" (e.g. generalized forces, heat fluxes, entropy flow vectors, etc.) which are consistent with the approximations underlying their conjugate variables.

In Section 3, we apply the relations developed in the preceding section to obtain a discrete description of the deformation and motion of non-polar media.

In Section 4 we list pertinent results of Coleman's thermodynamics of materials with memory [8], and recast certain of the basic equations in a form suitable for use in the construction of finite element models. In the following section, we focus our attention on a typical finite element of a continuum, on which we bring to bear the general thermodynamical equations and the general kinematical equations for finite elements developed previously. We then obtain general equations of motion, and heat conduction for a finite element of a nonlinear continua in terms of the generalized displacements, velocities and temperatures at discrete nodal points on the element. These equations pertain to a single element. Corresponding global equations governing the entire assembly of elements comprising the model, are obtained using a series of singular transformations.

We devote the final section of the paper to a discussion of some of the results obtained in the investigation.

Because of the important physical interpretations associated with simplicial approximations, an Appendix is included in which special attention is given to the simplex representations of the deformation of finite elements. These depict the deformation in a small finite element of the continuum as homogeneous and are derived easily from basic kinematic arguments.

2. THEORY OF FINITE ELEMENTS

We review here the concept of finite elements as a means of obtaining discrete models of continuous fields. Basic topological ideas are developed for spaces of dimension 3, but these can be easily generalized to spaces of higher dimension. Details on generalizations of the finite-element method can be found in [7].

Consider a closed region $\mathscr{R}$ of 3-dimensional Euclidean space $\mathscr{E}^3$. Points in $\mathscr{E}^3$ are denoted $\mathbf{x}$. We consider the region $\mathscr{R}$ to be the domain of a continuous single-valued function $\mathbf{T}(\mathbf{x})$

whose values may be scalars, vectors, or tensors of any order. By definition, the function $\mathbf{T}(\mathbf{x})$ associates with each of infinitely many points $\mathbf{x} \in \mathscr{R}$ a unique value T. The problem now considered is the following: Given $\mathbf{T}(\mathbf{x})$ and $\mathscr{R}$, construct an approximation of $\mathbf{T}(\mathbf{x})$ and $\mathscr{R}$ in which the function is characterized by a finite number of its values in $\mathscr{R}$. We proceed as follows:

(1) We identify a finite number G of points in $\mathscr{R}$ and label them consecutively $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_G$, or more concisely, $\mathbf{x}_\Delta (\Delta = 1, \ldots, G)$. These points are called *nodal points* or simply *nodes*. The finite set of nodal points is denoted $\mathscr{R}_\mathbf{x}$. We approximate the region $\mathscr{R}$ by another region $\bar{\mathscr{R}} \supset \mathscr{R}_\mathbf{x}$; The regions $\bar{\mathscr{R}}$ and $\mathscr{R}_\mathbf{x}$ may or may not coincide.

(2) We denote the values of $\mathbf{T}(\mathbf{x})$ at the nodal points $\mathbf{x}_\Delta \in \mathscr{R}$ by $\mathbf{T}_\Delta$:

$$\mathbf{T}_\Delta \equiv \mathbf{T}(\mathbf{x}_\Delta) \qquad \Delta = 1, 2, \ldots, G. \tag{2.1}$$

(3) We now consider a finite number E of disconnected subregions r_e of $\mathscr{E}^3$ called *finite elements*. Points belonging to a typical finite element r_e are denoted ξ or $\xi^{(e)}$ to distinguish them from points $\mathbf{x} \in \mathscr{R}$. Ultimately, we hope to connect all of the elements together to form $\bar{\mathscr{R}}$; but, at this point, all finite elements are considered closed and disjoint: the boundary of each element is distinct from that of all other elements. The union $\mathscr{R}^* = \bigcup_{e=1}^{E_e} r_e$ is referred to as the *disconnected* or *unassembled region*.

(4) We consider each finite element r_e to be the domain of a local field $\mathbf{t}^{(e)}(\xi)$, $\xi \in r_e$. The local fields are continuous within their respective finite elements. Of course, on connecting the elements together we intend for the local fields to form the original field $\mathbf{T}(\mathbf{x})$ over $\mathscr{R}$, but at this point the functions $\mathbf{t}^{(e)}(\xi)$ are considered to be unrelated to $\mathbf{T}(\mathbf{x})$ or to each other. Within each finite element, a finite number N_e of points are identified and are labeled consecutively $\xi_1^{(e)}, \xi_2^{(e)}, \ldots \xi_{N_e}^{(e)}$, or $\xi_N^{(e)} (N = 1, 2, \ldots, N_e)$. These points are called *local nodal points* or simply *local nodes*. The finite set of local nodal points is denoted $\mathscr{R}_\xi^*$.

(5) The values of $\mathbf{t}^{(e)}(\xi)$ at the local nodal points $\xi_N^{(e)} \in r_e$ are denoted $\mathbf{t}_N^{(e)}$:

$$\mathbf{t}_N^{(e)} \equiv \mathbf{t}^{(e)}(\xi_N^{(e)}). \tag{2.2}$$

(6) The local fields $\mathbf{t}^{(e)}(\xi)$ are approximated over their respective finite elements by functions of the form

$$\mathbf{t}^{(e)}(\xi) \approx \mathbf{t}^{(e)}(\xi) = \boldsymbol{\Psi}^{(e)}(\xi, \mathbf{t}_N^{(e)}) \tag{2.3}$$

where

$$\boldsymbol{\Psi}^{(e)}(\xi_M, \mathbf{t}_N^{(e)}) = \mathbf{t}_M^{(e)} \qquad \xi_M \in r_e. \tag{2.4}$$

The functions $\boldsymbol{\Psi}^{(e)}(\ )$ are defined only within r_e and are continuous within their respective finite elements. The functions $\boldsymbol{\Psi}^{(e)}(\ )$ are generalizations of the familiar Lagrange interpolation polynomials, though they need not be polynomials. In general, we take these functions to be linear in the nodal values $\mathbf{t}_N^{(e)}$:

$$\boldsymbol{\Psi}^{(e)}(\xi, \mathbf{t}_N^{(e)} = \overset{(e)}{\psi}{}^N(\xi)\mathbf{t}_N^{(e)} \tag{2.5}$$

wherein the repeated index N is to be summed from 1 to N_e. Here the scalar-valued functions $\overset{(e)}{\psi}{}^N(\xi)$ are such that

$$\overset{(e)}{\psi}{}^N(\xi_M) = \delta_M^N \qquad \xi_M \in r_e \tag{2.6}$$

where $\delta_M^N (N, M = 1, 2, \ldots, N_e)$ is the Kronecker delta.

(7) The connectivity of the model is established by mapping the global nodal points $\mathbf{x}_\Delta$ into the local points $\xi_N^{(e)}$ by the incidence relation

$$\xi_N^{(e)} = \overset{(e)}{\Omega}{}_N^\Delta \mathbf{x}_\Delta \tag{2.7}$$

with $N = 1, 2, \ldots, N_e$; $\Delta = 1, 2, \ldots, G$, where

$$\overset{(e)}{\Omega}{}_N^\Delta = \begin{cases} 1 & \text{if node } \xi_N^{(e)} \text{ of element } r_e \text{ is identical to node } \mathbf{x}_\Delta \text{ of the connected model.} \\ 0 & \text{if otherwise.} \end{cases} \tag{2.8}$$

Likewise, since one-to-one correspondences exist between $\mathbf{T}_\Delta$ and $\mathbf{x}_\Delta$ and $\mathbf{t}_N^{(e)}$ and $\xi_N^{(e)}$, we have

$$\overset{(e)}{\mathbf{t}}_N = \overset{(e)}{\Omega}{}_N^\Delta \mathbf{T}_\Delta. \tag{2.9}$$

Formally, we may regard (2.7) and (2.9) as the homomorphisms $\Omega: \mathscr{R}_\mathbf{x} \to \mathscr{R}_\xi^*$ and $\Omega: G \to L$, where G and L are global and local spaces, the elements of which are the sets of global values $\{\mathbf{T}_\Delta\}$ and the sets of pairs $\mathscr{L} = \sum_{e=1}^{E_e} \mathscr{L}_e$; $\mathscr{L}_e = \{\mathbf{y}: \mathbf{y} = (\mathbf{t}_N^{(e)}, \xi_N^{(e)})\}$ (see [7]). Since the identification of nodal points is arbitrary, (2.7) also implies the mapping $\Omega: \mathscr{R}^* \to \bar{\mathscr{R}}$. Transformations of the form in (2.7) and (2.9) were employed by Kron [9] in connection with network analysis, and form the basis of the "displacement method" of Argyris [10]. Oden [7] has indicated "compatibility conditions," necessary for the existence of these transformations, which insure that the proper correspondence prevails between the location of local element nodes and global nodal points in the connected model.

(8) The final finite-element approximation $\bar{\mathbf{T}}(\xi)$ of the field $\mathbf{T}(\mathbf{x})$ is given by

$$\mathbf{T}(\xi) = \sum_e \mathbf{t}^{(e)}(\xi) = \sum_e \overset{(e)}{\psi}{}^N(\xi) \overset{(e)}{\Omega}{}_N^\Delta \mathbf{T}_\Delta. \tag{2.10}$$

Ordinarily, the functions $\overset{(e)}{\psi}{}^N(\xi)$ are selected so that $\bar{\mathbf{T}}(\xi)$ is continuous across interelement boundaries in $\bar{\mathscr{R}}$. For ease in constructing functions $\overset{(e)}{\psi}{}^N(\xi)$ with properties (2.6) which, on connecting the elements together, make $\bar{\mathbf{T}}(\xi)$ continuous in $\bar{\mathscr{R}}$, the geometry of finite elements is usually selected to be very simple. For this reason, $\mathscr{R}$ and $\bar{\mathscr{R}}$ need not coincide. In an appendix, we consider simplicial approximations; that is, the fields $\mathbf{t}^{(e)}(\xi)$ are assumed to be linear in ξ and $N_e = k + 1$, k being the dimension of the space.

Conjugate fields

We also remark that in all applications of the finite-element method, the primary field $\mathbf{T}(\mathbf{x})$ which is to be approximated is accompanied by the following: (1) Another field $\mathbf{S}(\mathbf{x})$; (2) A scalar field $g(\mathbf{x}) = \mathbf{T}(\mathbf{x}) * \mathbf{S}(\mathbf{x})$, where $*$ denotes an operation which maps $\mathbf{T}(\mathbf{x})$ and $\mathbf{S}(\mathbf{x})$ into a scalar-valued function $g(x)$; and (3) a functional $Q[\mathbf{T}(\mathbf{x}), \mathbf{S}(\mathbf{x})]$ defined by

$$Q[\mathbf{T}(\mathbf{x}), \mathbf{S}(\mathbf{x})] = \int_{\mathscr{R}} \mathbf{T}(\mathbf{x}) * \mathbf{S}(\mathbf{x}) \, d\mathscr{R}. \tag{2.11}$$

We say that $\mathbf{S}(\mathbf{x})$ is conjugate to $\mathbf{T}(\mathbf{x})$ with respect to $Q[\mathbf{T}, \mathbf{S}]$. For the finite-element model, we have [7]

$$\bar{Q} = \sum_e \bar{q}^{(e)} = \mathbf{T}_\Delta * \mathbf{S}^\Delta = \sum_e \mathbf{t}_N^{(e)} * \mathbf{S}_e^N \tag{2.12}$$

where $\bar{Q}$ is the approximate value of the functional,

$$\mathbf{S}^{\Delta} = \sum_{e} {}^{(e)}\Omega^{\Delta}_{N}\mathbf{s}^{N}_{(e)} \tag{2.13}$$

and

$$\mathbf{s}^{N}_{(e)} \equiv \int_{r_e} {}^{(e)}\psi^{N}(\xi)\mathbf{s}^{(e)}(\xi)\,\mathrm{d}r_e. \tag{2.14}$$

Here $\mathbf{s}^{(e)}(\xi)$ is the portion of $\mathbf{S}(\mathbf{x})$ defined locally over r_e in the connected model. Notice that while (2.9) establishes a simple incidence relation between local and global values of the primary field, (2.13) indicates that the global value $\mathbf{S}^{\Delta}$ at node $\mathbf{x}_{\Delta}$ is obtained by summing all local values $\mathbf{s}^{N}_{(e)}$ at the local nodes incident on $\mathbf{x}_{\Delta}$ of all elements connected to that node in the final model of $\mathbf{T}(\mathbf{x})$. In (2.14) we say that $\mathbf{s}^{N}_{(e)}$ is the generalized nodal value of the conjugate field at node N of element e, consistent with the approximation $\bar{\mathbf{t}}^{(e)}(\xi)$.

3. KINEMATICS OF FINITE ELEMENTS

In this section we use the ideas developed in the previous section to describe the deformation and motion of finite elements of nonpolar media.

We consider a body $\mathscr{B}$ with material points X and identify the material point X with its place $\mathbf{X}$ in a fixed reference configuration $\boldsymbol{\varkappa}(\mathscr{B})$. The deformation of $\mathscr{B}$ from its reference configuration to its configuration at time t is described by a sufficiently smooth function

$$\mathbf{x} = \chi(\mathbf{X}, t) \tag{3.1}$$

where $\mathbf{x}$ denotes the point occupied by the particle X at time t.

The deformation gradient $\mathbf{F}$ at X and t is given by

$$\mathbf{F} = \nabla\chi(\mathbf{X}, t) \tag{3.2}$$

where ∇ is the gradient with respect to the fixed reference configuration. The velocity gradient $\mathbf{L}$ and the right and left Cauchy–Green tensors $\mathbf{B}$ and $\mathbf{C}$ are given by

$$\mathbf{L} = \dot{\mathbf{F}}\mathbf{F}^{-1}, \qquad \mathbf{B} = \mathbf{F}\mathbf{F}^{T}, \qquad \mathbf{C} = \mathbf{F}^{T}\mathbf{F} \tag{3.3}$$

where the superposed dot indicates a material time derivative and $(\ )^{T}$ indicates transposition.

We are particularly interested in the following form of the deformation function $\chi(X, t)$ in (3.1):

$$\chi(\mathbf{X}, t) = \mathbf{X} + \mathbf{U}(\mathbf{X}, t) \tag{3.4}$$

where $\mathbf{U}(\mathbf{X}, t)$ is the displacement of $\mathbf{X}$ relative to the reference configuration. It follows that

$$\mathbf{F} = \mathbf{I} + \mathbf{H} \tag{3.5}$$

where $\mathbf{I}$ is the unit tensor and $\mathbf{H} = \nabla\mathbf{U}$ is the displacement gradient. Corresponding expressions for $\mathbf{L}$, $\mathbf{B}$, and $\mathbf{C}$ in terms of $\mathbf{H}$ can be obtained by introducing (3.5) into (3.3).

The finite element

Following the scheme outlined in the previous section and noting that in this case $k = 3$, we suppose that the region $\boldsymbol{\varkappa}(\mathscr{B})$ occupied by the body $\mathscr{B}$ in the reference configuration is approximated by a collection of a finite number E of finite elements, connected appropriately together at a finite number G of places $\mathbf{X}_\Delta$ called nodes. Then, taking full advantage of the fundamental property of finite element models, we temporarily consider the elements to be disjoint and confine our attention to a typical finite element e. Element e corresponds to a region r_e which is the reference configuration of a portion B_e of the body $B: r_e = \boldsymbol{\varkappa}(\mathscr{B}_e)$. Points in r_e will be denoted by $\boldsymbol{\Xi}$ and the N_e local nodal points of the element will be denoted by $\boldsymbol{\Xi}_N (N = 1, 2, \ldots, N_e)$.

We now consider a localized deformation $\boldsymbol{\chi}^{(e)}$ of the element which carries the material points $\boldsymbol{\Xi}$ onto the current configuration in which points are denoted by $\boldsymbol{\xi}$, i.e.

$$\boldsymbol{\xi} = \boldsymbol{\chi}^{(e)}(\boldsymbol{\Xi}, t). \tag{3.6}$$

The local displacement vector over the element is then

$$\mathbf{u}^{(e)} = \boldsymbol{\xi} - \boldsymbol{\Xi}. \tag{3.7}$$

Recalling (2.9), we introduce the following local approximation of the displacement field $\mathbf{u}^{(e)}(\boldsymbol{\Xi}, t)$ over the element r_e:

$$\mathbf{u}^{(e)} = \mathbf{u}^{(e)}(\boldsymbol{\Xi}, t) = \psi^N(\boldsymbol{\Xi})\mathbf{u}_N^{(e)}(t) \tag{3.8}$$

where $\psi^N(\boldsymbol{\Xi})$ are defined in (2.10), $\mathbf{u}_N^{(e)}$ is the displacement at node N at time t, and the repeated index is to be summed from 1 to N_e. It follows that

$$\boldsymbol{\chi}^{(e)}(\boldsymbol{\Xi}, t) = \boldsymbol{\Xi} + \psi^N(\boldsymbol{\Xi})\mathbf{u}_N^{(e)}(t) \tag{3.9}$$

is the approximated deformation function. For the finite element then

$$\mathbf{H}^{(e)} = (\nabla\psi^N(\boldsymbol{\Xi}) \otimes \mathbf{u}_N^{(e)}(t))^T \tag{3.10}$$

$$\mathbf{F}^{(e)} = \mathbf{1} + (\nabla\psi^N(\boldsymbol{\Xi}) \otimes \mathbf{u}_N^{(e)}(t))^T. \tag{3.11}$$

In addition to the purely kinematical quantities, we approximate the local temperature field $\theta^{(e)}(\boldsymbol{\Xi}, t)$ over the element by

$$\theta^{(e)} = \theta^{(e)}(\boldsymbol{\Xi}, t) = \psi^N(\boldsymbol{\Xi})\theta_N^{(e)}(t) \tag{3.12}$$

where $\theta_N^{(e)}$ is the temperature at node N at time t.

With the local approximations given by (3.8) and (3.12), it is now a simple matter to connect the elements together and construct the complete finite-element representation of the displacement and temperature fields. Let $\boldsymbol{U}_\Delta$ and $\boldsymbol{\Theta}_\Delta$ denote the global values of displacement and temperature at node $\mathbf{X}_\Delta$ of the connected assembly of elements. Then according to (2.13),

$$\mathbf{u}_N^{(e)} = \overset{(e)}{\Omega}{}_N^\Delta \mathbf{U}_\Delta \qquad \theta_N^{(e)} = \overset{(e)}{\Omega}{}_N^\Delta \Theta_\Delta \tag{3.13}$$

and finally

$$\begin{aligned} \mathbf{U}(\boldsymbol{\Xi}, t) &= \sum_{e=1}^{E} \overset{(e)}{\Omega}{}_N^\Delta \psi^N(\boldsymbol{\Xi})\mathbf{U}_\Delta(t) \\ \Theta(\boldsymbol{\Xi}, t) &= \sum_{e=1}^{E} \overset{(e)}{\Omega}{}_N^\Delta \psi^N(\boldsymbol{\Xi})\Theta_\Delta(t). \end{aligned} \tag{3.14}$$

In an appendix, we demonstrate that a simplex approximation of the deformation of a continuous body depicts the local deformation within an element as a homogeneous deformation.

4. THERMODYNAMICS OF DISSIPATIVE MEDIA

According to Coleman [8], the free energy f of a simple dissipative material can be expressed as a functional of the total past history of deformation and temperature. Upon reduction for material frame indifference, this is written as

$$f = \overset{\infty}{\underset{s=0}{\varphi}}\,(C^t, \theta^t) \tag{4.1}$$

where, following Noll [11],

$$\mathbf{C}^t = \mathbf{C}(t-s) \qquad \theta^t = \theta(t-s). \tag{4.2}$$

The functional $\varphi(\ )$ is assumed to possess certain smoothness properties, the character of which is discussed by Coleman and Mizel [12].

In the following, we record the essential equations of Coleman's thermodynamical theory of simple materials [8], all pertinent quantities being with respect to the reference configuration $\kappa(\mathscr{B})$†:

I.
$$\bar{\mathbf{T}}_{(R)}(t) = 2\rho_{(R)} D_{\mathbf{C}} \overset{\infty}{\underset{s=0}{\varphi}}\,(\mathbf{C}^t, \theta^t) \tag{4.3}$$

$$\eta(t) = -D_\theta \overset{\infty}{\underset{s=0}{\varphi}}\,(\mathbf{C}^t, \theta^t) \tag{4.4}$$

where $\bar{\mathbf{T}}_{(R)}$ is the second Piola–Kirchhoff stress tensor, $\rho_{(R)}$ is the mass density in the reference configuration, η is the specific entropy, and D_C, D_θ are special operators defined in [13].

II.
$$\mathbf{h}_{(R)} = \overset{\infty}{\underset{s=0}{\mathbf{K}}}\,(\mathbf{C}^t, \theta^t, \nabla\theta) \tag{4.5}$$

where $\mathbf{h}_{(R)}$ is the heat flux vector referred to the reference configuration‡ and $\mathbf{K}(\ )$ is a vector-valued functional which possesses the same smoothness properties as $\varphi(\ )$.

III. The internal dissipation σ at time t corresponding to the pair of histories $(\mathbf{C}^t, \theta^t)$ is nonnegative and is obtained from $\varphi(\ )$ as follows:

$$\theta\sigma = -\delta_{\mathbf{C}^t} \overset{\infty}{\underset{s=0}{\varphi}} \left(\mathbf{C}^t, \theta^t \middle| \frac{d\mathbf{C}^t}{ds}\right) - \delta_{\theta^t} \overset{\infty}{\underset{s=0}{\varphi}} \left(\mathbf{C}^t, \theta^t \middle| \frac{d\theta^t}{ds}\right) \tag{4.6}$$

Here $\delta_{\mathbf{C}^t}\varphi$ and $\delta_{\theta^t}\varphi$ are the partial Frechet derivatives described by Coleman and Mizel [12] and the vertical stroke indicates that the functionals are linear in the quantity which follows; that is, $\delta_{\mathbf{C}^t}\varphi$ and $\delta_{\theta^t}\varphi$ are linear in $d\mathbf{C}^t/ds$ and $d\theta^t/ds$, respectively.

† We adopt here notation similar to that of Truesdell and Noll [13].

‡ The heat-flux functional $\mathbf{h}$ of Coleman [8] is not to be confused with the functional $\mathbf{K}$. The two functionals are related by

$$\overset{\infty}{\underset{s=0}{\mathbf{K}}}\,(\ ) = |\det \mathbf{F}|\mathbf{C}^{-1} \overset{\infty}{\underset{s=0}{\mathbf{h}}}\,(\ ).$$

IV. The dependence of $\mathbf{K}$ of (4.5) on the temperature gradient and histories $(\mathbf{C}^t, \theta^t)$ is such that

$$\mathbf{h}_{(R)} \cdot \nabla\theta + \rho_{(R)}\theta^2\sigma \geq 0. \tag{4.7}$$

In terms of the free energy f, the local balance of energy is

$$\rho_{(R)}\dot{f} + \rho_{(R)}\dot{\theta}\eta + \rho_{(R)}\theta\dot{\eta} = \operatorname{tr}(\bar{\mathbf{T}}_{(R)}\mathbf{F}^T\nabla\dot{\mathbf{u}}) + \operatorname{Div}\mathbf{h}_{(R)} + \rho_{(R)}r \tag{4.8}$$

where tr indicates the trace, $\mathbf{u}$ is the displacement vector with respect to the reference configuration, Div is the divergence operator with respect to the place $\mathbf{X}$ in $\boldsymbol{\kappa}(\mathscr{B})$, r is the heat supplied per unit mass, and

$$\dot{f} = 2\operatorname{tr}\left(\mathbf{F}D_{\mathbf{C}}\overset{\infty}{\underset{s=0}{\varphi}}(\mathbf{C}^t, \theta^t)\dot{\mathbf{F}}^T\right) + D_\theta\overset{\infty}{\underset{s=0}{\varphi}}(\mathbf{C}^t, \theta^t)\dot{\theta} - \theta\sigma. \tag{4.9}$$

The above results can be combined to obtain

$$\rho_{(R)}\theta\dot{\eta} - \operatorname{Div}\mathbf{h}_{(R)} - \rho_{(R)}r - \rho_{(R)}\theta\sigma = 0. \tag{4.10}$$

To the basic equations recorded above we may add Cauchy's first law of motion

$$\operatorname{Div}(\mathbf{F}\bar{\mathbf{T}}_{(R)}) + \rho_{(R)}\mathbf{b} = \rho_{(R)}\ddot{\mathbf{u}} \tag{4.11}$$

where $\mathbf{b}$ is the body force density.

5. FINITE ELEMENTS OF DISSIPATIVE MEDIA

Equations (4.3)–(4.11) describe a general theory of thermodynamics of simple media. We now derive two special global forms obtained from (4.10) and (4.11) that are of fundamental importance in deriving general equations of motion and heat conduction for finite elements of dissipative media.

Let $\delta\dot{\mathbf{u}}$ and $\delta\theta$ denote arbitrary instantaneous variations in the velocity and temperature of a body $\mathscr{B}$ at time t. Taking the inner product of (4.11) with $\delta\dot{\mathbf{u}}$ and multiplying (4.10) through by $\delta\theta$, we obtain the pair

$$\delta\dot{\mathbf{u}} \cdot \operatorname{Div}(\mathbf{F}\bar{\mathbf{T}}_{(R)}) + \rho_{(R)}\delta\dot{\mathbf{u}} \cdot \mathbf{b} = \rho_{(R)}\delta\dot{\mathbf{u}} \cdot \ddot{\mathbf{u}} \tag{5.1}$$

$$\rho_{(R)}\delta\theta\theta\dot{\eta} - \delta\theta \operatorname{Div}\mathbf{h} - \rho_{(R)}\delta\theta r - \rho_{(R)}\delta\theta\theta\sigma = 0. \tag{5.2}$$

Introducing the identities

$$\operatorname{Div}(\mathbf{F}\bar{\mathbf{T}}_{(R)}\delta\dot{\mathbf{u}}) = \delta\dot{\mathbf{u}} \cdot \operatorname{Div}(\mathbf{F}\bar{\mathbf{T}}_{(R)}) + \operatorname{tr}(\bar{\mathbf{T}}_{(R)}\mathbf{F}^T\nabla\delta\dot{\mathbf{u}}) \tag{5.3}$$

$$\operatorname{Div}(\delta\theta\mathbf{h}) = \delta\theta \operatorname{Div}\mathbf{h} + \mathbf{h} \cdot \nabla\delta\theta \tag{5.4}$$

and assuming suitable smoothness properties of the indicated variables, we employ the divergence theorem to obtain the global forms

$$\int_{\mathscr{P}} [\rho_{(R)}\ddot{\mathbf{u}} \cdot \delta\dot{\mathbf{u}} + \operatorname{tr}(\mathbf{T}_{(R)}\mathbf{F}^T\nabla\delta\dot{\mathbf{u}})]\, dv = \int_{\mathscr{P}} \rho_{(R)}\delta\dot{\mathbf{u}} \cdot \mathbf{b}\, dv + \int_{\partial\mathscr{P}} \mathbf{t}_{(R)} \cdot \delta\dot{\mathbf{u}}\, dS_{(R)} \tag{5.5}$$

and

$$\int_{\mathscr{P}} [\rho_{(R)}\theta\delta\theta\dot{\eta} + \mathbf{h}_{(R)} \cdot \nabla\delta\theta - \rho_{(R)}\theta\delta\theta\sigma]\, dv = \int_{\mathscr{P}} \rho_{(R)} r\delta\theta\, dv + \int_{\delta\mathscr{P}} \delta\theta \mathbf{h}_{(R)} \cdot \mathbf{n}_{(R)}\, dS_{(R)} \quad (5.6)$$

where $\mathscr{P}$ is the part of the body under consideration, $\partial\mathscr{P}$ is its boundary, $\mathbf{t}_{(R)}$ is the surface traction referred to a surface area $dS_{(R)}$ in the reference configuration, and $\mathbf{n}_{(R)}$ is a unit vector normal to $dS_{(R)}$. Equations (5.5) and (5.6) may be considered to be general virtual work principles for continuous media. For thermomechanically simple media, (5.5) and (5.6) become

$$\int_{\mathscr{P}} \rho_{(R)}\ddot{\mathbf{u}} \cdot \delta\dot{\mathbf{u}}\, dv + \int_{\mathscr{P}} 2\rho_{(R)} \operatorname{tr}(D_{\mathbf{C}} \overset{\infty}{\underset{s=0}{\varphi}} (\mathbf{C}^t, \theta^t)\mathbf{F}^T \nabla\delta\dot{\mathbf{u}})\, dv = \int_{\mathscr{P}} \rho_{(R)}\delta\dot{\mathbf{u}} \cdot \mathbf{b}\, dv + \int_{\partial\mathscr{P}} \mathbf{t}_{(R)} \cdot \delta\dot{\mathbf{u}}\, dS_{(R)} \quad (5.7)$$

$$\int \left[\rho_{(R)}\theta\delta\theta \overset{\infty}{\underset{s=0}{\mathscr{G}}} (\mathbf{C}^t, \theta^t) + \nabla\delta\theta \cdot \overset{\infty}{\underset{s=0}{\mathbf{K}}} (\mathbf{C}^t, \theta^t, \nabla\theta) + \rho_{(R)}\delta\theta \sum_{s=0}^{\infty} \left(\mathbf{C}^t, \theta^t \left| \frac{d\mathbf{C}^t}{dS}, \frac{d\theta^t}{ds} \right| \right) \right] dv = \int_{\mathscr{P}} r\delta\theta\rho_{(R)}\, dv + \int_{\partial\mathscr{P}} \delta\theta \mathbf{h}_{(\dot{R})} \mathbf{n}_{(R)}\, ds_{(R)} \quad (5.8)$$

where, for simplicity, we have denoted

$$\overset{\infty}{\underset{s=0}{\mathscr{G}}} (\mathbf{C}^t, \theta^t) = \overset{\cdot}{\overline{-D_\theta \overset{\infty}{\underset{s=0}{\varphi}} (\mathbf{C}^t, \theta^t)}}$$

$$= -2 \operatorname{tr}\left[\mathbf{F} D_{\mathbf{C}} D_\theta \overset{\infty}{\underset{s=0}{\varphi}} (\mathbf{C}^t, \theta^t)\dot{\mathbf{F}}^T \right] + D_\theta^2 \overset{\infty}{\underset{s=0}{\varphi}} (\mathbf{C}^t, \theta^t)\dot{\theta} \quad (5.9)$$

$$+ \delta_{\mathbf{C}_r^t} D_\theta \overset{\infty}{\underset{s=0}{\varphi}} (\mathbf{C}^t, \theta^t | d\mathbf{C}^t/ds) + \delta_{\theta_r^t} D_\theta \overset{\infty}{\underset{s=0}{\varphi}} (\mathbf{C}^t, \theta^t | d\theta^t/ds)$$

$$\sum_{s=0}^{\infty} \left(\mathbf{C}^t, \theta^t \left| \frac{d\mathbf{C}^t}{ds}, \frac{d\theta^t}{ds} \right| \right) = -\delta_{\mathbf{C}_r^t} \overset{\infty}{\underset{s=0}{\varphi}} (\mathbf{C}^t, \theta^t | d\mathbf{C}^t/ds) - \delta_{\theta_r^t} \overset{\infty}{\underset{s=0}{\varphi}} (\mathbf{C}^t, \theta^t | d\theta^t/ds). \quad (5.10)$$

Motion of a finite element

We now consider the body $\mathscr{B}$ to be a collection of a finite number E of discrete elements $\mathscr{B}_{(e)}$ as described in Sections 2 and 3. Taking advantage of the fundamental property of finite-element models, we isolate a typical finite element $\mathscr{B}_{(e)}$ and consider its behavior under the motion and temperature fields described in Section 3. Accordingly, a material description of the velocity and temperature fields over the element is given by

$$\dot{\mathbf{u}} = \psi^N(\Xi)\dot{\mathbf{u}}_N^{(e)} \qquad \theta = \psi^N(\Xi)\theta_N^{(e)} \quad (5.11)$$

where $\psi^N(\Xi)$ are the interpolation functions defined in (2.6) and $\mathbf{u}_N^{(e)}$ and $\theta_N^{(e)}$ are the time-dependent displacement and temperature at node N of element e. Instantaneous variations in these local fields at time t are clearly

$$\delta\dot{\mathbf{u}} = \psi^N(\Xi)\delta\dot{\mathbf{u}}_N^{(e)} \qquad \delta\theta = \psi^N(\Xi)\delta\theta_N^{(e)}. \quad (5.12)$$

Introducing $(5.12)_1$ into (5.7) and simplifying, we obtain

$$\left\{m_{(e)}^{NM}\ddot{\mathbf{u}}_M^{(e)} + \int_{\mathscr{P}_{(e)}} 2\rho_{(R)} \overset{\infty}{\underset{s=0}{\hat{\boldsymbol{\varphi}}}}(\Xi, \overset{(e)}{\mathbf{u}_K^t}, \overset{(e)}{\theta_K^t})\nabla\psi^N(\Xi)\,dv + \int_{\mathscr{P}_{(e)}} [2\rho_{(R)}\mathbf{u}_M^{(e)} \cdot \overset{\infty}{\underset{s=0}{\hat{\varphi}}}(\Xi, \overset{(e)}{\mathbf{u}_K^t}, \overset{(e)}{\theta_K^t})\nabla\psi^M(\Xi)]\nabla\psi^N(\Xi)\,dv - \mathbf{p}_{(e)}^N\right\} \cdot \delta\dot{\mathbf{u}}_N^{(e)} = 0 \tag{5.13}$$

where

$$m_{(e)}^{NM} = \int_{\mathscr{P}_{(e)}} \rho_{(R)}\psi^N(\Xi)\psi^M(\Xi)\,dv \tag{5.14}$$

$$\mathbf{p}_{(e)}^N = \int_{\mathscr{P}_{(e)}} \rho_{(R)}\psi^N(\Xi)\mathbf{b}\,dv + \int_{\partial\mathscr{P}_{(e)}} \psi^N(\Xi)\mathbf{t}_{(R)}\,ds_{(R)} \tag{5.15}$$

$$\overset{\infty}{\underset{s=0}{\hat{\boldsymbol{\varphi}}}}(\Xi, \overset{(e)}{\mathbf{u}_K^t}, \overset{(e)}{\theta_K^t}) = D_{\mathbf{C}} \overset{\infty}{\underset{s=0}{\varphi}}(\overset{(e)}{\mathbf{C}^t(\mathbf{u}_K^{(e)})}, \overset{(e)}{\theta^t(\theta_K^{(e)})}). \tag{5.16}$$

The array $m_{(e)}^{NM}$ is the consistent mass matrix for the element, $\mathbf{p}_{(e)}^N$ is the generalized force at node N, and $\hat{\boldsymbol{\varphi}}(\,)$ is a functional of the histories of the nodal displacements and temperatures. The significance of these quantities is discussed more fully in the following section.

Returning to (5.13), we observe that this energy balance for the element must hold for arbitrary variations $\delta\dot{\mathbf{u}}_N^{(e)}$ in the nodal velocities (and as a consequence of the property of the inner product of a vector $\mathbf{a}$ and an arbitrary vector $\mathbf{b}$, $\mathbf{a} \cdot \mathbf{b} = 0 \Rightarrow \mathbf{a} = \mathbf{0}$), the quantity in braces must vanish, and we extract from (5.13) the *general equations of motion for a finite element of a thermodynamically simple media*:

$$m_{(e)}^{NM}\ddot{\mathbf{u}}_M^{(e)} + \int_{\mathscr{P}_{(e)}} 2\rho_{(R)} \overset{\infty}{\underset{s=0}{\hat{\boldsymbol{\varphi}}}}(\Xi, \overset{(e)}{\mathbf{u}_K^t}, \overset{(e)}{\theta_K^t})\nabla\psi^N(\Xi)\,dv + \int_{\mathscr{P}_{(e)}} [2\rho_{(R)}\mathbf{u}_M^{(e)} \cdot \overset{\infty}{\underset{s=0}{\hat{\varphi}}}(\Xi, \overset{(e)}{\mathbf{u}_K^t}, \overset{(e)}{\theta_K^t})\nabla\psi^M(\Xi)]\nabla\psi^N(\Xi)\,dv = p_{(e)}^N(t). \tag{5.17}$$

Again, diagonally repeated nodal indices are to be summed from 1 to N_e.

Heat conduction in a finite element

Substituting (5.12) into (5.8) and simplifying, we get

$$\left\{\int_{\mathscr{P}_{(e)}} \rho_{(R)}\left[\psi^N(\Xi)\psi^M(\Xi)\theta_M^{(e)} \overset{\infty}{\underset{s=0}{\hat{\mathscr{G}}}}(\Xi, \overset{(e)}{\mathbf{u}_K^t}, \overset{(e)}{\theta_K^t}) + \psi^N(\Xi) \overset{\infty}{\underset{s=0}{\hat{\sum}}}(\Xi, \overset{(e)}{\mathbf{u}_K^t}, \overset{(e)}{\theta_K^t})\right] dv + \int_{\mathscr{P}_{(e)}} \nabla\psi^N(\Xi) \cdot \overset{\infty}{\underset{s=0}{\hat{\mathbf{K}}}}(\Xi, \overset{(e)}{\mathbf{u}_K^t}, \overset{(e)}{\theta_K^t})\,dv - q_{(e)}^N\right\}\delta\theta_N^{(e)} = 0 \tag{5.18}$$

where

$$\overset{\infty}{\underset{s=0}{\hat{\mathscr{G}}}}(\Xi, \overset{(e)}{\mathbf{u}_K^t}, \overset{(e)}{\theta_K^t}) = \overset{\infty}{\underset{s=0}{\mathscr{G}}}(\overset{(e)}{\mathbf{C}^t(\mathbf{u}_K^{(e)})}, \overset{(e)}{\theta^t(\theta_K^{(e)})}) \tag{5.19}$$

$$\overset{\infty}{\underset{s=0}{\hat{\sum}}}(\Xi, \overset{(e)}{\mathbf{u}_K^t}, \overset{(e)}{\theta_K^t}) = \sum_{s=0}^{\infty}(\overset{(e)}{\mathbf{C}^t(\mathbf{u}_K^{(e)})}, \overset{(e)}{\theta^t(\theta_K^{(e)})}) \tag{5.20}$$

$$\overset{\infty}{\underset{s=0}{\hat{\mathbf{K}}}}(\Xi, \overset{(e)}{\mathbf{u}_K^t}, \overset{(e)}{\theta_K^t}) = \overset{\infty}{\underset{s=0}{\mathbf{K}}}(\overset{(e)}{\mathbf{C}^t(\mathbf{u}_K^{(e)})}, \overset{(e)}{\theta^t(\theta_K^{(e)})}, \nabla\psi^N(\Xi)\theta_N^{(e)} \tag{5.21}$$

and

$$q^N_{(e)} = \int_{\mathscr{P}_{(e)}} \rho_{(R)} \psi^N(\Xi) r \, dv + \int_{\partial\mathscr{P}_{(e)}} \psi^N(\Xi) \mathbf{h}_{(R)} \cdot \mathbf{n}_{(R)} \, ds_{(R)}. \tag{5.22}$$

The functionals defined in (5.13)–(5.21) represent the entropy production internal dissipation, and heat flux for the finite element. We observe that each involves only the histories $(\overset{(e)}{u^t_N}, \overset{(e)}{\theta^t_N})$ of the nodal values of the displacement and temperature. Note that due to the character of the local temperature field over the element, the dependence of $\overset{\infty}{\underset{s=0}{\mathbf{K}}}(\,)$ on the temperature gradient history is reflected in only a dependence on the histories of the nodal temperatures $\overset{(e)}{\theta^t_K}$ in $\overset{\infty}{\underset{s=0}{\hat{\mathbf{K}}}}(\,)$. In (5.22) the quantity $q^N_{(e)}$ represents a generalized normal component of heat flux at node N of element e. Further properties of these functionals and generalized fluxes are discussed in Section 6 of this paper.

Since (5.18) must hold for arbitrary variations $\delta\theta^{(e)}_N$ in the nodal temperatures, the quantity in braces must vanish, and we arrive at the *general equations of heat conduction for a finite element of a thermodynamically simple media*:

$$\begin{aligned}\int_{\mathscr{P}_{(e)}} \rho_{(R)} \Bigg[\psi^M(\Xi)\psi^N(\Xi)\theta^{(e)}_M \overset{\infty}{\underset{s=0}{\hat{\mathscr{G}}}}(\Xi, \overset{(e)}{\mathbf{u}^t_K}, \overset{(e)}{\theta^t_K}) + \psi^N(\Xi) \sum_{s=0}^{\infty} (\Xi, \overset{(e)}{\mathbf{u}^t_K}, \overset{(e)}{\theta^t_K}) \Bigg] dv \\ + \int_{\mathscr{P}_{(e)}} \nabla\psi^N(\Xi) \overset{\infty}{\underset{s=0}{\hat{\mathbf{K}}}}(\Xi, \overset{(e)}{\mathbf{u}^t_K}, \overset{(e)}{\theta^t}) \, dv = q^N_{(e)}(t) \, .\end{aligned} \tag{5.23}$$

Global forms

Equations (5.17) and (5.23) represent the equations of motion and heat conduction for a single finite element. To obtain the corresponding equations for the entire collection of elements, all connected appropriately together to form the complete discrete model of the media, we must introduce the notion of global values of the fields $\mathbf{u}(\Xi, t)$ and $\theta(\Xi, t)$ and the mappings $\Omega: \mathscr{G} \to \mathscr{L}$ described in (3.13) and (3.14).

Let $\mathbf{P}^\Delta$ and $Q^\Delta (\Delta = 1, 2, \ldots, G)$ denote the global values of generalized force and heat flux at node Δ of the connected system of elements. Then, since $\mathbf{P}(\Xi, t)$ and $Q(\Xi, t)$ are conjugate to $\mathbf{u}(\Xi, t)$ and $\theta(\Xi, t)$, respectively, we have, according to (2.17),

$$\mathbf{P}^\Delta = \sum \overset{(e)}{\Omega^\Delta_N} \mathbf{p}^N_{(e)} \qquad Q^\Delta = \sum \overset{(e)}{\Omega^\Delta_N} q^N_{(e)}. \tag{5.24}$$

Introducing (5.17) and (3.13) into $(5.24)_1$, we obtain

$$M^{\Delta\Gamma} \dot{\mathbf{U}}^t_\Gamma + \overset{\infty}{\underset{s=0}{\mathbf{\Phi}^\Delta}}(\mathbf{U}^t_\Gamma, \Theta^t_\Gamma) + \overset{\infty}{\underset{s=0}{\mathbf{\Psi}^{\Delta\Gamma}}}(\mathbf{U}^t_\gamma, \Theta^t_\gamma)\mathbf{U}_\Gamma = P^\Delta(t) \tag{5.25}$$

where

$$M^{\Delta\Gamma} = \sum_e \overset{(e)}{\Omega^\Delta_N} m^{NM}_{(e)} \overset{(e)}{\Omega^\Gamma_M} \tag{5.26}$$

$$\overset{\infty}{\underset{s=0}{\mathbf{\Phi}^\Delta}}(\mathbf{U}^t_\Gamma, \Theta^t_\Gamma) = \sum \overset{(e)}{\Omega^\Delta_N} \int_{\mathscr{P}_{(e)}} 2\rho^{(e)}_{(R)} \nabla\psi^N(\Xi) \overset{\infty}{\underset{s=0}{\hat{\mathbf{\Phi}}}}(\Xi, \overset{(e)}{\Omega^\Gamma_K}\mathbf{U}^t_\Gamma, \overset{(e)}{\Omega^\Gamma_K}\Theta^t_\Gamma) \, dv \tag{5.27}$$

$$\overset{\infty}{\underset{s=0}{\mathbf{\Psi}^{\Delta\Gamma}}}(\mathbf{U}^t_\Omega, \Theta^t_\Omega) = \sum_e \overset{(e)}{\Omega^\Delta_N} \overset{(e)}{\Omega^\Gamma_M} \int_{\mathscr{P}_{(e)}} 2\rho^{(e)}_{(R)} \operatorname{tr}\Bigg[\overset{\infty}{\underset{s=0}{\hat{\mathbf{\Phi}}}}(\Xi, \overset{(e)}{\Omega^\gamma_K}\mathbf{U}^t_\gamma, \overset{(e)}{\Omega^\gamma_K}\Theta^t_\gamma) \Delta\psi^N(\Xi) \otimes \Delta\psi^M(\Xi) \Bigg] dv \tag{5.28}$$

Here $M^{\Delta\Gamma}$ is the "mass matrix" for the entire assembly of elements, and $\Phi(\,)$ and $\Psi(\,)$ are functionals to the $2G$ histories $\mathbf{U}^t_\Delta$ and Θ^t_Δ of the nodal displacements and temperatures.

Equation (5.25) is the final equation(s) of motion of the assembly of finite elements. Boundary and initial conditions are applied by merely prescribing the nodal displacement $\mathbf{U}_\Delta$ or force $\mathbf{P}_\Delta$ at boundary nodes, or by prescribing initial values of these quantities at global nodal points.

Turning now to the heat conduction equations, we introduce (5.23) and (3.14) into $(5.24)_2$ and obtain

$$\overset{\infty}{\underset{s=0}{G^{\Delta\Gamma}}}(\mathbf{U}^t_\Upsilon, \Theta^t_\Upsilon)\Theta_\Gamma + \overset{\infty}{\underset{s=0}{S^{\Delta}}}(\mathbf{U}^t_\Upsilon, \Theta^t_\Upsilon) + \overset{\infty}{\underset{s=0}{H^{\Delta}}}(\mathbf{U}^t_\Upsilon, \Theta^t_\Upsilon) = Q^\Delta(t) \tag{5.29}$$

where

$$\overset{\infty}{\underset{s=0}{G^{\Delta\Gamma}}}(\mathbf{U}^t_\Upsilon, \Theta^t_\Upsilon) = \sum_e \overset{(e)}{\Omega}{}^\Delta_N \overset{(e)}{\Omega}{}^\Gamma_M \int_{\mathscr{P}_{(e)}} \rho^{(e)}_{(R)} \left[\psi^N(\Xi)\psi^M(\Xi) \overset{\infty}{\underset{s=0}{\hat{\mathscr{G}}}}(\Xi, \overset{(e)}{\Omega}{}^\Upsilon_K \mathbf{U}^t_\Upsilon, \overset{(e)}{\Omega}{}^\Upsilon_K \Theta^t_\Upsilon)\right] d\upsilon \tag{5.30}$$

$$\overset{\infty}{\underset{s=0}{S^{\Delta}}}(\mathbf{U}^t_\Upsilon, \Theta^t_\Upsilon) = \sum_e \overset{(e)}{\Omega}{}^\Delta_N \int_{\mathscr{P}_{(e)}} \psi^N(\Xi) \sum_{s=0}^{\infty} (\Xi, \overset{(e)}{\Omega}{}^\Upsilon_K \mathbf{U}^t_\Upsilon, \overset{(e)}{\Omega}{}^\Upsilon_K \Theta^t_\Upsilon)\, d\upsilon \tag{5.31}$$

$$\overset{\infty}{\underset{s=0}{H^{\Delta}}}(\mathbf{U}^t_\Upsilon, \Theta^t_\Upsilon) = \sum_e \overset{(e)}{\Omega}{}^\Delta_N \int_{\mathscr{P}_{(e)}} \nabla\psi^N(\Xi) \overset{\infty}{\underset{s=0}{\hat{\mathbf{K}}}}(\Xi, \overset{(e)}{\Omega}{}^\Upsilon_K U^t_\Upsilon, \overset{(e)}{\Omega}{}^\Upsilon_K \Theta^t_\Upsilon)\, d\upsilon. \tag{5.32}$$

Here $G(\,)$, $S(\,)$ and $H(\,)$ are functionals of the $2G$ histories $\mathbf{U}^t_\Delta$ and Θ^t_Δ of the nodal displacements and temperatures.

Equation (5.29) is the final equation of heat conduction for the assembly of finite elements.

6. DISCUSSION

The terms appearing in the equations of motion and heat conduction admit to interesting physical interpretation. As noted previously, the array $m^{NM}_{(e)}$ of (5.14) is the consistent mass matrix for finite element e [14]. The array $M^{\Delta\Gamma}$ of (5.25) is its counterpart for the entire assembly of elements. Physically $m^{NM}_{(e)}$ represents a generalized "inertia-force" at node N due to a unit (virtual) acceleration at node M, $\delta\ddot{\mathbf{u}}^{(e)}_M = \mathbf{I}$. The array $m^{NM}_{(e)}$ reflects the manner in which the total mass of an element is to be distributed to each node so that the total kinetic energy of the element is consistent with the approximate acceleration field $\psi^N(\Xi)\ddot{\mathbf{u}}^{(e)}_N$.

The force $\mathbf{p}^N_{(e)}$ of (5.15) represents the generalized force at node N of element e, computed so as to be consistent with the velocity field $\psi^N(\Xi)\mathbf{u}^{(e)}_N$ over the element. In general, $\mathbf{p}^N_{(e)}$ can be decomposed into a part due to body forces and a part due to surface tractions:

$$\mathbf{p}^N_{(e)} = \mathbf{b}^N_{(e)} + \mathbf{t}^N_{(e)} \tag{6.1}$$

where, according to (5.15),

$$\mathbf{b}^N_{(e)} = \int_{\mathscr{P}_{(e)}} \rho_{(R)}\psi^N(\Xi)\mathbf{b}\, d\upsilon \qquad \mathbf{t}^N_{(e)} = \int_{\mathscr{P}_{(e)}} \psi^N(\Xi)\mathbf{t}_{(R)}\, ds_{(R)}. \tag{6.2}$$

Now the term $\mathbf{p}^N_{(e)} \cdot \delta\dot{\mathbf{u}}^{(e)}$ in (5.13) represents the mechanical power $P_{(e)}$ of the element developed by the external forces. Thus, $\mathbf{b}$ and $\mathbf{t}_{(R)}$ are conjugate to the velocity field $\delta\dot{\mathbf{u}}^{(e)}$ with respect to the mechanical power of the element. It follows that $\mathbf{b}^N_{(e)}$ and $\mathbf{t}^N_{(e)}$ are

concentrated forces lumped at nodes N of element e in such a way as to develop the same mechanical power as the distributed body forces $\mathbf{b}(\Xi, t)$ and tractions $\mathbf{t}_{(R)}(\Xi, t)$.

In $(6.2)_2$ we observe that the calculation of the forces $\mathbf{t}^N_{(e)}$ involves integration over a surface element $dS_{(R)}$ with outward unit normal $\mathbf{n}_{(R)}$ in the reference configuration. The tractions $\mathbf{t}$, however, are usually available to us only in the current configuration and it becomes necessary to relate the current surface element ds to the element $ds_{(R)}$ as follows [13]:

$$ds = \sqrt{(J\mathbf{n}_{(R)} \cdot \mathbf{C}^{-1}\mathbf{n}_{(R)})}\, ds_{(R)} \tag{6.3}$$

where $\mathbf{C}^{-1}$ is the inverse of the deformation tensor in $(3.3)_3$ and

$$J = |\det \mathbf{F}| = \sqrt{\det \mathbf{C}}. \tag{6.4}$$

Similar calculations are required in computing the generalized heat fluxes in (5.22). In this regard, note that in addition to being able to prescribe either a generalized heat flux or temperature at boundary nodes, it is also possible to consider boundary-layer effects for the finite-element model. The procedure outlined by Oden and Kross [15] for linear thermoelasticity is applicable in this case provided that the current surface element and its orientation is related to the reference configuration in the manner indicated above.

To interpret the global forces $\mathbf{P}^\Delta$ in $(5.24)_1$, note that the total variation in mechanical power of the collection of elements due to the instantaneous local variations $\delta\dot{\mathbf{u}}^e_N$ is

$$\delta P = \mathbf{P}^\Delta \cdot \delta\dot{\mathbf{U}}_\Delta = \sum_e \delta P_{(e)} \tag{6.5}$$

where $\delta P_{(e)} = \mathbf{p}^N_{(e)} \cdot \delta\dot{\mathbf{u}}^{(e)}_N$ and $\delta\dot{\mathbf{u}}^{(e)}_N = \overset{(e)}{\Omega}{}^\Delta_N \delta\dot{\mathbf{U}}_\Delta$. Thus, for arbitrary variations $\delta\dot{\mathbf{U}}_\Delta$ in the nodal velocities

$$(\mathbf{P}^\Delta - \sum_e \overset{(e)}{\Omega}{}^\Delta_N \mathbf{p}^N_{(e)}) \cdot \delta\mathbf{U}_\Delta = 0. \tag{6.6}$$

Therefore, $(5.24)_1$ follows from the fact that the total mechanical power of the disjoint elements developed by instantaneous variations in the nodal velocities is the same as that of the connected assembly of finite elements.

In view of (6.1) and $(5.24)_1$, it is clear that

$$\mathbf{P}^\Delta = \mathbf{B}^\Delta + \mathbf{T}^\Delta \tag{6.7}$$

where

$$\mathbf{B}^\Delta = \sum_e \overset{(e)}{\Omega}{}^\Delta_N \mathbf{b}^N_{(e)} \qquad \mathbf{T}^\Delta = \sum_e \overset{(e)}{\Omega}{}^\Delta_N \mathbf{t}^N_{(e)}. \tag{6.8}$$

The local nodal force $\mathbf{t}^N_{(e)}$ of $(6.2)_2$ is the analog of stress in the discrete model of the continuum. Consequently, on assembling the collection of finite elements into a single discrete model of the entire body $\mathscr{B}$, the local values $\mathbf{t}^N_{(e)}$ play the role of contact forces and sum vectorially to zero at interior (global) nodal points. Thus $\mathbf{T}^\Delta$ is zero except at nodal points on the boundary. The forces $\mathbf{B}^\Delta$, however, exist at the nodes of all elements in which body forces are present.

Equation (5.16) reflects the fact that the histories $(\mathbf{C}^t, \theta^t)$ for a finite element are uniquely determined by the histories of the nodal values of displacement and temperature. Hence, the functional $D_{\mathbf{C}} \overset{\infty}{\underset{s=0}{\varphi}}(\,)$ can be reduced to a functional of $(\overset{(e)}{\mathbf{u}}{}^t_K, \overset{(e)}{\theta}{}^t_K)$. The dependence on Ξ can be eliminated by integration over the volume of the element once a specific form of $\overset{\infty}{\underset{s=0}{\varphi}}(\,)$ has been identified.

The question of convergence cannot be thoroughly explored until specific forms of the reduced constitutive functionals [e.g. (5.30)–(5.32)] have been specified. However, mean convergence of $\bar{\mathbf{u}}^e, \bar{\theta}^e$ to $\mathbf{u}$ and θ can be guaranteed, independent of the form of these functionals, provided the well-known completeness and continuity requirements are met (cf. [16]–[18]). For example, since $\mathbf{u}(\mathbf{x}, t)$ is continuous and finite everywhere and $\mathbf{u}^{(e)}_N \equiv \mathbf{u}(\boldsymbol{\xi}^{(e)}_N, t)$, $\mathbf{u}(\mathbf{x}, t)$ is bounded in r_e. Thus, with $\|\mathbf{u}\|^2 = \int_r \mathbf{u} \cdot \mathbf{u}\, dr$, there is positive M such that $\|\mathbf{u} - \mathbf{u}^e_N\| \leq M$. Likewise, for arbitrary $\boldsymbol{\xi} \in r_e$, $\|\mathbf{u} - \boldsymbol{\psi}^N(\boldsymbol{\xi})\mathbf{u}^e_N\| < K$ where K depends on M. Since $\boldsymbol{\psi}^N(\boldsymbol{\xi})$ are complete and are selected so that $\bar{\mathbf{u}}(\boldsymbol{\xi}, t)$ is continuous, it is clear that both M and K can be made arbitrarily small if the network of elements is appropriately refined (see Synge [16] or Key [17]). While the more important problem of convergence of, say $\|\bar{\mathscr{F}}(\bar{\mathbf{u}})\| \to \|\mathscr{F}(\mathbf{u})\|$, $\mathscr{F}(\,)$ being a nonlinear operator, cannot be rigorously resolved, definite statements can be made concerning special cases of (5.25) and (5.29). For example, in the case of small deformations of a hyperelastic solid, (5.25) reduces to the well-known finite element equations derived from minimum potential energy considerations. Thus, our model appears to provide a lower bound to the energy, at least in this case. Moreover, from a physical viewpoint and in view of the assumed smoothness of the integrands in (5.5) and (5.6), convergence of θ and $\mathbf{u}$ appears likely in very general cases due to the fact that each is uniquely defined within an element by a simplex approximation (see the Appendix) which arises physically by expanding the temperature and deformation about some reference state.

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REFERENCES

[1] M. A. BIOT, *Phys. Rev.* **97**, 1463–1469 (1955).
[2] M. A. BIOT, *J. appl. Phys.* **25**, 1385–1391 (1954).
[3] M. A. BIOT, *J. appl. Phys.* **27**, 240–253 (1956).
[4] M. J. TURNER, R. W. CLOUGH, H. C. MARTIN and L. P. TOPP, *J. aeronaut. Sci.* **23**, 805–823, 854 (1956).
[5] O. C. ZIENKIEWICZ and Y. K. CHEUNG, *The Finite Element Method in Structural and Continuum Mechanics*. McGraw-Hill (1967).
[6] J. T. ODEN, *Developments in Theoretical and Applied Mechanics*. Pergamon (1968).
[7] J. T. ODEN, *J. numer.-Methods Engng* **1**, 205–221 (1969).
[8] B. D. COLEMAN, *Archs. ration. Mech. Analysis* **17**, 1–46 (1964).
[9] G. KRON, *Tensor Analysis of Networks*. Wiley (1939).
[10] J. H. ARGYRIS, *Energy Theorems and Structural Analysis*. Butterworth (1960).
[11] W. NOLL, *Archs. ration. Mech. Analysis* **2**, 197 (1958).
[12] B. D. COLEMAN and V. J. MIZEL, *Archs. ration. Mech. Analysis* **27**, 255 (1967).
[13] C. TRUESDELL and W. NOLL, The non-linear field theories of mechanics. In: *Flügge's Handbuch der Physik*, Vol. III/3. Springer (1965).
[14] J. S. ARCHER, *AIAA Jnl.* **3**, 1910–1918 (1965).
[15] J. T. ODEN and D. A. KROSS, *Proc. 2nd Conf. Matrix Meth. St. Mech.* Wright-Patterson Air Force Base, Ohio (1968).
[16] J. L. SYNGE, *The Hypercircle in Mathematical Physics*, Cambridge University Press (1957).
[17] S. W. KEY, Ph.D. Dissertation, University of Washington, Seattle (1966).
[18] E. R. DE ARANTES E OLIVEIRA, *Int. J. Solids Struct.* **4**, 929–952 (1968).

APPENDIX

Homogenous deformations and temperature fields

An important case of the general finite element which has been described in Section 3 is obtained if we choose topological simplexes for finite elements [6, 7]. A simplex element in three-dimensional space has four vertices ($N_e = 4$) and may be regarded as a tetrahedron. The importance of this element does not lie totally in the fact that they are geometrically as well as algebraically simple, rather, it has to do with the physical significance of the simplex approximation.

Consider a three-dimensional simplex finite element, r_e, with nodal points $\Xi_N (N = 1, 2, 3, 4)$ in the reference configuration. The approximation of the local deformation $\chi^{(e)}$ will be made by assuming $\chi^{(e)}$ to be homogeneous, i.e.

$$\xi = \chi^{(e)}(\Xi, t) = \xi_0(t) + \mathbf{F}^{(e)}(t)(\Xi - \Xi_0) \tag{A.1}$$

where Ξ_0 is a point in $\kappa(\mathscr{B}_e)$, $\xi_0 = \chi^{(e)}(\Xi_0, t)$, and $\mathbf{F}^{(e)}(t)$ is a second order non-singular tensor.

The objective is to express the tensor $\mathbf{F}^{(e)}$ in terms of nodal values. To this end the point Ξ_0 in (A.1) is identified with the node labeled 4. It follows that

$$\mathbf{D}(\Xi) = \Xi - \Xi_4, \qquad \mathbf{d}(\xi) = \xi - \xi_4 \tag{A.2}$$

are respectively the position vectors relative to mode 4 for the point $\Xi \in \kappa(\mathscr{B}_e)$ and the point $\xi \in \chi^{(e)}(\mathscr{B}_e, t)$. Until further notice all primed indices will have the range 1, 2, 3. Introduce at node 4 in $\kappa(\mathscr{B}_e)$ a set of three independent directors $\mathbf{D}_{N'}$ defined by

$$\mathbf{D}_{N'} = \mathbf{D}(\Xi_{N'}). \tag{A.3}$$

It can be seen that the $\mathbf{D}_{N'}$ are the position vectors relative to node 4 for the nodes 1, 2, 3 and are therefore known geometrical entities.

The deformation carries $\mathbf{D}_{N'}$ onto the $\mathbf{d}_{N'}$ which are the position vectors relative to node 4 of nodes 1, 2, 3 in the spatial configuration, i.e.

$$\mathbf{d}_{N'}(t) = \mathbf{F}^{(e)}(t)\mathbf{D}_{N'}. \tag{A.4}$$

Reciprocal directors $\mathbf{D}^{N'}$, $\mathbf{d}^{N'}$ can be introduced through the definition

$$\mathbf{D}^{N'} \cdot \mathbf{D}_{M'} = \delta^{N'}_{M'}, \qquad \mathbf{d}^{N'} \cdot \mathbf{d}_{M'} = \delta^{N'}_{M'}. \tag{A.5}$$

It can easily be shown that the deformation gradient $\mathbf{F}^e$, its inverse, and the right Cauchy–Green tensor $\mathbf{C}^{(e)}$ are given by

$$\begin{aligned} &\mathbf{F}^{(e)}(t) = \mathbf{d}_{N'}(t) \otimes \mathbf{D}^{N'}, \qquad \overset{-1}{\mathbf{F}}{}^{(e)}(t) = \mathbf{D}_{N'} \otimes \mathbf{d}^{N'}(t). \\ &\mathbf{C}^{(e)}(t) = d_{N'M'}(t)\mathbf{D}^{N'} \otimes \mathbf{D}^{M'} \end{aligned} \tag{A.6}$$

where $d_{N'M'} = \mathbf{d}_{N'} \cdot \mathbf{d}_{M'}$. The velocity field is

$$\dot{\xi} = \mathbf{v}(\xi, t) = \mathbf{v}_4(t) + (\mathbf{d}(\xi) \cdot \mathbf{d}^{N'}(t))\dot{\mathbf{d}}_{N'}(t) \tag{A.7}$$

where $\mathbf{v}_4$ is the velocity of node 4.

We may also choose to write the velocity field in terms of Lagrangian functions $\Psi^N(\xi)$

($N = 1, 2, 3, 4$) defined over $\chi^{(e)}(B_e, t)$, in which case

$$\mathbf{v}(\xi, t) = \Psi^N(\xi)\mathbf{v}_N(t) \tag{A.8}$$

where

$$\Psi^{N'}(\xi) = \mathbf{d}(\xi) \qquad \mathbf{d}^{N'} \sum_{N=1}^{4} \Psi^N(\xi) = 1. \tag{A.9}$$

Recall from (2.6) that $\Psi^N(\xi_M) = \delta^N_M$. Also

$$\mathbf{d}(\xi) \cdot \mathbf{d}^{N'} = \mathbf{D}(\Xi) \cdot \mathbf{D}^{N'}. \tag{A.10}$$

Thus, the velocity field can also be written in terms of Lagrangian functions $\Psi^N(\xi)$ defined over $\kappa(\mathscr{B}_e)$:

$$\mathbf{v}(\Xi, t) = \Psi^N(\Xi)\mathbf{v}_N(t) \tag{A.11}$$

where

$$\Psi^{N'}(\Xi) = \mathbf{D}(\Xi) \cdot \mathbf{D}^{N'}, \qquad \sum_{N=1}^{4} \Psi^N(\Xi) = 1. \tag{A.12}$$

Let $\mathbf{u}_N$ denote the value of the displacement field at the nodes. Then considering that $\dot{\mathbf{u}}_N = \mathbf{v}_N$ and $\mathbf{u}_N(0) = \mathbf{0}$ we have

$$\mathbf{u}(\Xi, t) = \Psi^N(\Xi)\mathbf{u}_N(t). \tag{A.13}$$

Also in view of $(A.2)_1$ and (A.13) the displacement gradient $\mathbf{H}^{(e)}$ is obtained as

$$\mathbf{H}^{(e)}(t) = \mathbf{u}_N(t) \otimes \boldsymbol{\varphi}^N \tag{A.14}$$

where

$$\boldsymbol{\varphi}^{N'} = \mathbf{D}^{N'}, \qquad \boldsymbol{\varphi}^4 = -\sum_{N=1}^{3} \mathbf{D}^{N'}. \tag{A.15}$$

The right Cauchy–Green tensor for the finite element is given by

$$\mathbf{C}^{(e)}(t) = \mathbf{1} + \mathbf{u}_N(t) \otimes \boldsymbol{\varphi}^N + \boldsymbol{\varphi}^N \otimes \mathbf{u}_N(t) + (\mathbf{u}_N(t) \cdot \mathbf{u}_M(t))\boldsymbol{\varphi}^N \otimes \boldsymbol{\varphi}^M. \tag{A.16}$$

Let us now consider the local temperature field $\theta^e(\xi, t)$ which we approximate over $\chi^{(e)}(\mathscr{B}_e, t)$ by

$$\theta(\xi, t) = \theta_4(t) + \mathbf{g}(t) \cdot \mathbf{d}(\xi) \tag{A.17}$$

where $\theta_4(t)$ is the temperature at node 4 and $\mathbf{g}(t)$ is a time-dependent vector independent of ξ given by

$$\mathbf{g}(t) = \theta_{N'}(t)\mathbf{d}^{N'} - \theta_4(t) \sum_{N'=1}^{3} \mathbf{d}^{N'}. \tag{A.18}$$

Here $\theta_{N'}(t)$ is the temperature of nodes 1, 2, 3. We may also choose to write the temperature θ in terms of Lagrangian functions $\Psi^N(\xi)$, $\Psi^N(\Xi)$, in which case

$$\theta(\xi, t) = \Psi^N(\xi)\theta_N(t), \qquad \theta(\Xi, t) = \Psi^N(\Xi)\theta_N(t). \tag{A.19}$$

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Абстракт—Работа касается развития общих дискретных моделей, способных вполне описать общее термомеханическое поведение широкого класса нелинейных материалов с запоминанием. Используются общие концепции конечного элемента, в связи с термодинамикой простых материалов Колемана, для получения уравнений движения и теплопроводности для конечных элементов нелинейных континуумов. Определяется кинематика конечных элементов в общих выражениях, специально учитывая идею, что локально однородные деформации и поля температуры равны симплексным приближениям сделанным на элементе. Проверяются некоторые уравнения термодинамической теории материалов Колемана, используя их для разработки ураьнений, касающихся поведения типичного конечного элемента. Не дается никаких ограничений, касающихся градиентов деформации или градиентов температуры. Приводятся топологические свойства совокупности таких элементов для построения плотных, дискретных моделей диссипативнвх сред с произвольной геометрией, начальными и граничными условиями.