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FE THERMOMECHANICS AND MATERIAL SAMPLING POINTS

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The thermomechanics of finite elements of continuous media is discussed. The novel key concept introduced is that of material sampling points attributed to each finite element. Similar to representing the spatial interactions by a finite number of nodal quantities, the state of a finite element is represented by the set of local states at its sampling points. The fully algebraic, thermomechanical equations of the discrete model are formulated using Biot's variational approach. The constitutive description in this finite element theory pertains to formulating the constitutive equations locally at all sampling points. A linear elasticity problem and a heat conduction problem illustrate the theory.

1. Introduction

The almost common view today on finite element discretizations for continuum flow and deformation problems regards the finite element method as a mere mathematical tool for obtaining approximate solutions of the governing differential equations. Within each element an approximation of the actual solution is sought within the class of interpolation polynomials of typically low degree on the basis of the nodal values. Commonly, an associated functional, obtained usually by Galerkin's method, then provides the system of generally nonlinear algebraic matrix equations for the unknown nodal quantities.

Except for the simplest elements, the matrices obtained involve rather complicated integrals which are commonly evaluated by numerical integration. Although it seems in the spirit of this view on finite element techniques to aim at minimization of the errors introduced in the numerical integration process, it has been frequently noted that a reduced order of integration may actually improve the accuracy and convergence of the approximate solution.

The author shares the opinion expressed for instance by Besseling [2, 3] that it might be doubted whether the mathematical formulation of the physical problem in terms of functional analysis without taking due note of the underlying physical concepts is indeed a fruitful starting point. As distinct from the above viewpoint, the finite element approach presented in this paper is best characterized as a direct discrete description of continuum thermomechanics. Rather than starting out from the standard continuum description in terms of differential field equations, we return in this approach to the most primitive of continuum thermomechanical concepts and we derive, by consideration of the thermomechanical behaviour of finite elements of the continuous medium, the discrete analogues of these field equations.

Following the lines proposed by Biot [4], the balances of mass and of entropy supplemented with a virtual energy balance are adopted as the basic principles of thermomechanics. The

continuum model is based upon the theory of the natural reference state [1, 5]. As compared with the approach of e.g. Besseling [3], the essential novel feature of the present approach is the concept of so-called material sampling points. This concept is believed to complete the analogy between the continuum field theory and the discrete, finite element theory. The main line of thinking in this approach will be exemplified by considering quadratic spatial elements that may be used e.g. in a spatial description of two-dimensional thermomechanical process.

In this paper, we shall use Cartesian tensor components (termed tensors for simplicity) denoted with subscripts i, j , or k as indices. The standard summation convention applies to repeated tensor indices. A superposed dot denotes the material time derivative. Superscripts m and n are used to indicate a nodal point number; superscripts r and s indicate a sampling point number. Component vectors (or simply vectors) are denoted in bold-face type. Matrices are denoted with (light-face) capitals, unless stated otherwise. In addition to standard vector operations, a special vector product is used which is defined as follows: Let $\mathbf{a}$ and $\mathbf{b}$ be n -dimensional vectors, $\mathbf{a} = [a^\alpha]^\mathbf{t}$, $\mathbf{b} = [b^\alpha]^\mathbf{t}$, $\alpha = 1, \dots, n$; the product $\mathbf{c} := \mathbf{a}\mathbf{b}$ then is a n -dimensional vector with components $c^\alpha = a^\alpha b^\alpha$ (no summation!).

2. Geometry

The construction of a finite element model of a body essentially consists of two main steps. Firstly, the actual corpuscular material is replaced with a continuous medium. Secondly, the continuous body is replaced with a connected set of finite elements of the continuum.

The so-called *simplex element* constitutes the discrete analogue of the infinitesimal volume element (cf. with Cauchy's infinitesimal tetrahedron in treatises on stresses). A simplex element in a p -dimensional physical (Euclidean) space $\mathcal{S}^p$, $1 \leq p \leq 3$, may be characterized by the set C^e of coordinates x_i^c , $i = 1, \dots, p$, of its $p + 1$ vertices. The set of all E elements, connected at common vertices and characterized by C^e , $e = 1, \dots, E$, determines the *discrete configuration* C of the body. It should be observed that by using simplex elements, the actual configuration can at any instant be approximated to any desired degree of accuracy.

Just as in continuum field theory, one may distinguish between material and spatial finite element descriptions. In a material description, the elements are distinct material bodies which are being transported through space. In a spatial description on the other hand, the elements are fixed in space, with matter being transported through the elements. As opposed to the former, the latter approach is particularly appropriate for problems of large deformations or flow.

The present finite element theory will be exemplified by a spatial description of two-dimensional thermomechanical processes by means of (triangular) simplex elements. For future reference, we introduce for these elements ($p = 2$) the vector of coordinate differences with components g_i^c , $i = 1, \dots, p$, $c = 1, \dots, p + 1$, defined by,

$$g_i^1 = e_{ij}(x_j^2 - x_j^3), \quad g_i^2 = e_{ij}(x_j^3 - x_j^1), \quad g_i^3 = e_{ij}(x_j^1 - x_j^2), \quad (2.1)$$

with e_{ij} the permutation symbol ($e_{11} = e_{22} = 0$, $e_{12} = 1$, $e_{21} = -1$).

3. Flow of mass and of entropy

For the macroscopic description of thermomechanical processes, the flow of mass and the flow of entropy are the two primitive concepts. The flow of the continuous matter in space is governed by the velocity field v_i , while, similarly, the flow of entropy through the medium is governed by the entropy flux field $\dot{h}_i$. The interactions of any (sub-) body with its surroundings are represented by the fields of velocity and entropy flux along with their energetically dual fields.

The essence of the finite element theory is contained in the observation that knowledge of the flow of mass and of entropy is adequate in a phenomenological sense, if it is available in a finite number of points of the continuum. An approximation of the velocity and entropy flux fields may be obtained by interpolating locally between the values in these points.

For simplex elements in $\mathcal{S}^p$, the most simple interpolation functions are polynomials of degree 1. Such polynomials are members of the $(p+1)$ -dimensional vector space $\mathcal{P}_1^p$ (the vector space of all polynomials on a p -dimensional space of degree $\leq d$ is $\mathcal{P}_d^p$). Interpolation functions of higher degree d may also be applied, and are members of $\mathcal{P}_d^p$ with $d \geq 1$. Elements utilizing interpolation functions of degree d are termed *dth-order elements*. The required number of basis points for the interpolation is equal to the dimension of $\mathcal{P}_d^p$, as given by (see e.g. [7]),

$$\dim \mathcal{P}_d^p = \frac{(p+d)!}{p!d!} = \binom{p+d}{d}.$$

When applying such interpolations to the fields of velocity and entropy flux inside a simplex element, the values of these quantities at the boundary of the element are described by polynomials $\in \mathcal{P}_d^{p-1}$. In order to meet the basic continuum requirements of continuity of mass and entropy, continuity is to be ensured at element boundaries. This is accomplished by locating at each of the $p+1$ faces of the element $\dim \mathcal{P}_d^{p-1}$ basis points common with the adjacent element (for this reason, the basis points for the interpolation of velocity and entropy flux fields are termed nodal points). For each face, the p vertices are obvious candidates for nodal points. The position of the remaining boundary nodal points, as well as the position of the $\dim \mathcal{P}_d^p - \dim \mathcal{P}_d^{p-1}$ nodal points in the interior is arbitrary, but may be established by recalling that the faces of a simplex in $\mathcal{S}^p$ are simplices in $\mathcal{S}^{p-1}$ and by invoking the geometric symmetry properties of the simplex. The elements thus obtained are members of the family of Lagrange simplex elements (cf. e.g. [8]).

In this discrete description, the flow of mass and of entropy within a d th-order element in $\mathcal{S}^p$ is described by n^e -dimensional vectors v_i and $\dot{h}_i$, $i = 1, \dots, p$, of the velocity and entropy flux components at the n^e nodal points, $v_i = [v_i^n]^t$, $\dot{h}_i = [\dot{h}_i^n]^t$, $n = 1, \dots, n^e$, with n^e according to

$$n^e = \binom{p+d}{d}.$$

The rate of exchange of energy of the element with its surroundings accompanying the flow of mass and of entropy is composed of the mechanical power $\dot{W}^e$ of the forces exerted on the boundary of the element and the rate of heat supply $\dot{Q}$ through the boundary. In the

continuum model, these are given by $\dot{W}^e = \int t_i v_i \, dA$ and $\dot{Q} = - \int T n_i \dot{h}_i \, dA$, with t_i the traction vector field at the boundary, n_i the outer unit normal vector, and T the temperature of the surroundings. For each element, the exchange of energy now defines two component vectors $\mathbf{t}_i$ and $\mathbf{T}_i$ of nodal forces and nodal contact temperatures dual to $\mathbf{v}_i$ and $\dot{\mathbf{h}}_i$, respectively, such that

$$\dot{W}^e = \mathbf{t}_i^t \mathbf{v}_i, \quad \dot{Q} = - \mathbf{T}_i^t \dot{\mathbf{h}}_i, \quad (3.1)$$

at any instant. In this discrete description, the spatial interactions inside the continuum are thus represented by finite-dimensional vectors rather than by continuous fields.

For the spatial description of two-dimensional thermomechanical processes we will take a quadratic interpolation for velocity and entropy flux. The quadratic element then contains

$$n^e = \binom{4}{2} = 6$$

(spatially fixed) nodal points, located at the 3 vertices and at the midpoints of the 3 edges (see Fig. 1). Within the element, the fields of velocity and entropy flux may be interpolated according to

$$v_i(x_k, t) = \sum_{n=1}^6 v_i^n(t) \psi_n(\zeta_k), \quad \dot{h}_i(x_k, t) = \sum_{n=1}^6 \dot{h}_i^n(t) \psi_n(\zeta_k),$$

with the quadratic interpolation function being given by

$$[\psi_n(\zeta_k)]^t = [(2\zeta_1 - 1)\zeta_1, (2\zeta_2 - 1)\zeta_2, (2\zeta_3 - 1)\zeta_3, 4\zeta_1\zeta_2, 4\zeta_2\zeta_3, 4\zeta_3\zeta_1], \quad (3.2)$$

Fig. 1. Two-dimensional quadratic element.

where the ζ_k 's are the natural coordinates of a point inside the element (see Fig. 1),

$$\zeta_k = \frac{A_k}{A}, \quad \sum_{k=1}^3 \zeta_k = 1.$$

4. The concept of material sampling points

Under the influence of the interactions with the surrounding elements, the thermodynamic state of the continuous medium contained within an element will be subject to continuous change during the process. Similar to the assertion that knowledge of the flow of mass and of entropy is sufficient in a phenomenological sense if it is available in a finite number of points, we now assert that it is also sufficient to have the information on the thermodynamic state available in a finite number of points. These points may be regarded as points in which the material and its state are locally sampled, for which reason we will refer to them as *material sampling points*.

In addition to the nodal points, we now attribute to each finite element, being a distinct thermodynamic system, a number of such sampling points. Instead of by a field $q = q(x_i, t)$, any thermodynamic quantity q is represented by a vector of the values of q at the sampling points. An approximation of the field inside the element may in turn be obtained again by interpolation between the sampling point values. In a sense, the material sampling points in this discrete description replace the familiar material points in continuum theory.

It is essential to realize that the concept of material sampling points is fundamentally different from that of nodal points. In the nodal points, external (typically vectorial) quantities are defined that represent the interactions between adjacent elements. In the material sampling points on the other hand, internal quantities are defined, such as mass density and specific entropy, which characterize the local state of the material within the element. Being physically entirely different entities, nodal points and material sampling points will play an entirely different role in this finite element model.

Given an element and its nodal points, the question arises of how many sampling points should be applied per element and where they should be located. First of all, it should be realized that there is no point in adopting interpolations of the state quantities of higher degree than that induced through the interpolation used in the description of the flow of mass and of entropy. The local changes of the mass density and the specific entropy are to a large extent determined by the local divergence of the velocity and entropy fields. Having adopted interpolations of degree d for these latter fields, both divergence fields are described by polynomials of degree $d - 1$. Hence, it follows that the number of material sampling points attributed to each element must be such that interpolation functions can be completely described of one degree lower than that of the interpolation functions adopted for the description of the flow of mass and of entropy. From the discussion in Section 3, it is then deduced that *the number of material sampling points s^e within each d th-order element in $\mathcal{S}^p$ should be equal to*

$$s^e = \binom{p + d - 1}{d - 1}. \quad (4.1)$$

Before addressing the determination of the location of the material sampling points, let us briefly consider the description of the mass distribution. Rather than by a mass density field $\rho = \rho(x_i, t)$, the mass distribution in the discrete finite element model is represented by the s^e mass densities $\rho^s = \rho^s(t)$, $s = 1, \dots, s^e$, in the material sampling points of the element. Analogous to the field description in which the mass of any subbody is being given by $\int \rho \, dV$, the mass of the element is evaluated by the weighted sum $\sum_{s=1}^{s^e} \rho^s V^s$, with V^s the volume fractions attributed to each sampling point. These volume fractions are as yet unknown, but are related to the position of the sampling points. As a generalization, we may further define element inertia quantities of order k in the discrete and field descriptions by

$$I_{i_1, \dots, i_k}^d := \sum_s \rho^s x_{i_1} \cdots x_{i_k} V^s, \quad I_{i_1, \dots, i_k}^f := \int \rho x_{i_1} \cdots x_{i_k} \, dV,$$

respectively, $i = 1, \dots, p$, $n = 1, \dots, k$. The zeroth-order inertia is the mass of the element.

It is now asserted that the location of the material sampling points within each element, as well as the corresponding volume fractions, is determined by the following conditions:

- (1) *Each sampling point is located in the interior of the element.*
- (2) *The position of the sampling points respects the geometric symmetries of the element.*
- (3) *For any element of order d , the identity*

$$I_{i_1, \dots, i_k}^d \equiv I_{i_1, \dots, i_k}^f \quad \forall \rho^s, s = 1, \dots, s^e, \quad (4.2)$$

must hold for all $0 \leq k \leq d - 1$, where $\rho(x_i, t)$ is the approximation of the mass density field given by

$$\rho(x_i, t) = \sum_s \rho^s(t) \varphi_s(x_i), \quad (4.3)$$

with $\varphi_s(x_i)$ denoting the interpolation functions of degree $d - 1$ for the sampling point quantities.

The motivation for the first requirement lies in the very concept of material sampling points: In the sampling points, the material contained within the finite element as a distinct thermomechanical system is locally sampled. It is noted that this implies that the field approximations on the basis of the sampling point quantities are in general not continuous at interelement boundaries. The second requirement expresses the fact that in sampling the state of the material, we do not wish to bias one sampling point over the other.

The third requirement is connected with the two main steps in constructing a finite element model of a body as mentioned in Section 2. In replacing the actual corpuscular matter with a continuous medium, each infinitesimal—and in finite element terminology, linear—volume element of the continuum is attributed a mass density equal to the local macroscopic mass per unit volume of the actual material. This ensures identical zeroth-order macroscopic inertia properties of the actual body and the continuum model. Analogously, the third requirement above ensures for each d th-order finite element identical inertia properties of order up to and including $d - 1$ of the continuum and the finite element model.

Now, each element involves ps^e unknown sampling point coordinates and s^e unknown volume fractions. The assertion made here is that the three requirements stated are sufficient

to establish the position of the sampling points inside the element. However, all attempts to prove this in general have failed so far.

Let us now demonstrate this procedure for the second-order element in $\mathcal{S}^2$ introduced in the previous section. According to (4.1) this element contains

$$s^e = \binom{3}{1} = 3$$

spatially fixed material sampling points. When locating these points symmetrically with respect to the three edges, their position in natural coordinates is given by $(\lambda_1, \lambda_2, \lambda_3)$, $(\lambda_2, \lambda_3, \lambda_1)$, and $(\lambda_3, \lambda_1, \lambda_2)$, while the volume fractions satisfy $V^1 = V^2 = V^3$. For the application of the conditions (4.2), we need explicit expressions for the interpolation functions $\varphi_s(x_i)$ in (4.3) expressed in terms of the unknown sampling point coordinates $\lambda_1, \lambda_2, \lambda_3$. It is left to the reader to verify that these interpolation functions can be written as

$$[\varphi_s(\zeta_i)] = \frac{1}{\Delta} \begin{bmatrix} \zeta_1(\lambda_2\lambda_3 - \lambda_1^2) + \zeta_2(\lambda_3\lambda_1 - \lambda_2^2) + \zeta_3(\lambda_1\lambda_2 - \lambda_3^2) \\ \zeta_1(\lambda_3\lambda_1 - \lambda_2^2) + \zeta_2(\lambda_1\lambda_2 - \lambda_3^2) + \zeta_3(\lambda_2\lambda_3 - \lambda_1^2) \\ \zeta_1(\lambda_1\lambda_2 - \lambda_3^2) + \zeta_2(\lambda_2\lambda_3 - \lambda_1^2) + \zeta_3(\lambda_3\lambda_1 - \lambda_2^2) \end{bmatrix},$$

with Δ defined by,

$$\Delta = 3(\lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_3\lambda_1) - 1. \quad (4.4)$$

From the conditions (4.2) for $k=0$ then follows that $V^1 = V^2 = V^3 = \frac{1}{3}A$, while for $k = d-1 = 1$ it yields three equations for λ_1, λ_2 , and λ_3 , the first one of which reads,

Fig. 2. The position of the material sampling points in the two-dimensional quadratic element. The dashed curve represents the solution of (4.6).

$$4\Delta\lambda_1 + 2(\lambda_1^2 - \lambda_2\lambda_3) + (\lambda_2^2 - \lambda_3\lambda_1) + (\lambda_3^2 - \lambda_1\lambda_2) = 0, \quad (4.5)$$

provided $\Delta \neq 0$, the other two being given through cyclic interchange of the indices. It follows from (4.4) that $\Delta = 0$ only in the center of the element, $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$. Craftily invoking the property $\sum_i \lambda_i = 1$, it may be shown that the three equations indicated in (4.5) are equivalent with the single equation,

$$\lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_3\lambda_1 = \frac{1}{4}. \quad (4.6)$$

This equation describes the ellipse¹ inside the element that coincides with the boundary at the midpoints of the edges (see Fig. 2). According to the third requirement, the sampling points can be located anywhere on this ellipse. Complete symmetry is obtained, however, only if the coordinates of these three points satisfy the three properties $\lambda_2 = \lambda_3$, $\lambda_3 = \lambda_1$, and $\lambda_1 = \lambda_2$, respectively. Invoking then the first requirement, that the sampling points should be located in the interior of this element, it follows from (4.6) that they are located at $(\frac{2}{3}, \frac{1}{6}, \frac{1}{6})$, $(\frac{1}{6}, \frac{2}{3}, \frac{1}{6})$, and $(\frac{1}{6}, \frac{1}{6}, \frac{2}{3})$.

5. The discrete equations of thermomechanics

5.1. Material rates in a spatial description

In a spatial field description the material rate of change $\dot{q}$ of any physical quantity $q = q(x_i, t)$ is given by

$$\dot{q} = \frac{\partial q}{\partial t} + v_k \frac{\partial q}{\partial x_k}. \quad (5.1)$$

In this discrete description, the material rate of change of a sampling point quantity q^s is evaluated by local application of (5.1). Towards this end, an approximation of the local gradient of q at the sampling point is obtained from the field approximation $q(x_i, t) = \sum_s q^s(t) \varphi_s(x_i)$ within the element. For each element, then, with the vector $\mathbf{q}$ being defined by $\mathbf{q} = [q^s]^t$, $s = 1, \dots, s^e$, the discrete analogue of (5.1) reads,

$$\dot{\mathbf{q}} = \frac{\partial \mathbf{q}}{\partial t} + \mathbf{V}_k \nabla_k \mathbf{q}, \quad (5.2)$$

with $\mathbf{V}_k$ the vector of velocity components at the sampling points evaluated by interpolation between the nodal velocities,

$$\mathbf{V}_k := \mathbf{B} \mathbf{v}_k, \quad (5.3)$$

and ∇_k the $s^e \times s^e$ matrix determined by the gradient of the interpolation functions. For the quadratic two-dimensional element, these matrices are given by,

¹ This particular ellipse is known as Steiner's ellipse (± 1820).

$$B = \frac{1}{9} \begin{bmatrix} 2 & -1 & -1 & 4 & 1 & 4 \\ -1 & 2 & -1 & 4 & 4 & 1 \\ -1 & -1 & 2 & 1 & 4 & 4 \end{bmatrix},$$

$$A\nabla_k = \begin{bmatrix} g_k^1 & g_k^2 & g_k^3 \\ g_k^1 & g_k^2 & g_k^3 \\ g_k^1 & g_k^2 & g_k^3 \end{bmatrix}, \quad k = 1, 2,$$

with the g_k^e being defined in (2.1).

In the case of a linear element, the field approximation on the basis of the single material sampling point quantity does not provide a suitable approximation of the gradient. This may then be evaluated from the sampling point values in the $p + 1$ adjacent elements.

5.2. Rates of deformation, strain, and rotation

In the field description, the rate of deformation of the continuum is governed by a tensor field $L_{ij} = L_{ij}(x_k, t)$ given by

$$L_{ij} := \frac{\partial v_i}{\partial x_j}, \quad (5.4)$$

such that

$$\dot{\overline{dx}}_i = L_{ij} dx_j, \quad (5.5)$$

for any line element dx_i in an infinitesimal material neighbourhood of x_k . In the finite element model, now consider at each material sampling point s an infinitesimal neighbourhood $\mathcal{N}^s$ and an arbitrary material line element dx_i^s . Through local application of (5.4), (5.5) at each sampling point, we then find for each element

$$\dot{\overline{dx}}_i = L_{ij} dx_j, \quad (5.6)$$

where $\mathbf{dx}_i = [dx_i]^t$, $s = 1, \dots, s^e$, and the vector of the deformation rate tensors at the sampling points, $\mathbf{L}_{ij} = [L_{ij}^s]^t$, $s = 1, \dots, s^e$, is given by

$$\mathbf{L}_{ij} := \mathbf{D}_j \mathbf{v}_i. \quad (5.7)$$

The $s^e \times n^e$ matrix $\mathbf{D}_i$ is determined by the gradient of the interpolation functions for the velocities. For the quadratic element in $\mathcal{S}^2$ one derives from (3.2),

$$2A\mathbf{D}_i = \frac{1}{3} \begin{bmatrix} 5g_i^1 & -g_i^2 & -g_i^3 & 2(g_i^1 + 4g_i^2) & 2(g_i^2 + g_i^3) & 2(4g_i^3 + g_i^1) \\ -g_i^1 & 5g_i^2 & -g_i^3 & 2(4g_i^1 + g_i^2) & 2(g_i^2 + 4g_i^3) & 2(g_i^3 + g_i^1) \\ -g_i^1 & -g_i^2 & 5g_i^3 & 2(g_i^1 + g_i^2) & 2(4g_i^2 + g_i^3) & 2(g_i^3 + 4g_i^1) \end{bmatrix}, \quad i = 1, 2. \quad (5.8)$$

Decomposing each sampling point rate of deformation tensor in its symmetric and antisymmetric parts, we can define vectors D_{ij} and W_{ij} of strain-rate tensors and spin tensors such that,

$$D_{ij} = \frac{1}{2}(L_{ij} + L_{ji}), \quad W_{ij} = \frac{1}{2}(L_{ij} - L_{ji}). \quad (5.9)$$

In a discrete sense, the vectors L_{ij} , D_{ij} , and W_{ij} describe the rates of deformation, strain, and rotation of each finite element. They constitute $l^e = p^2 s^e$, $d^e = \frac{1}{2} p(p+1) s^e$, and $w^e = \frac{1}{2} p(p-1) s^e$ independent quantities, respectively. On the other hand, since an element in $\mathcal{S}^p$ allows for p translations and $\frac{1}{2} p(p-1)$ rotations as a rigid body, the n^e nodal velocities v_i^n define $p(n^e - 1)$ rate of deformation possibilities and $p(n^e - \frac{1}{2}(p+1))$ strain rate possibilities. A straightforward calculation shows that these numbers never exceed l^e and d^e , respectively. This ensures that all possible rates of deformation and strain-rates of the element can indeed be characterized by the vectors L_{ij} and D_{ij} .

5.3. Materials possessing a natural reference state

In this paper, we shall address in particular the thermomechanics of materials possessing a so-called *natural reference state*. A recent reformulation of the continuum model and the constitutive theory for such materials as originally introduced by Besseling [1] has been effected by Van der Giessen [5]. In spite of its simple structure, the theory of the natural reference state has been shown to provide nonlinear constitutive models for a wide range of material behaviour from gases to highly deformable elastoplastic solids [6]. It is outside the scope of the present paper to discuss the concept of the natural reference state in detail; the reader is referred to the above-mentioned references.

In the present sampling point approach, the concept of the natural reference state is enunciated through the following:

(1) For the material neighbourhood $\mathcal{N}^s$ of any material sampling point s there exists at any instant a fixed physical reference state: *The natural reference state*. This implies that the physical properties of the material currently at this sampling point in the natural reference state are preserved during the process. The anisotropic properties may be defined with respect to a Cartesian triad $\{\epsilon_\alpha^s\}$ with fixed directions in space attached to $\mathcal{N}^s$.

(2) A line element dx_i^s in $\mathcal{N}^s$ in the actual current state is at any instant related to the corresponding line element da_α^s in the natural reference state by the invertible transformation,

$$dx_i^s = c_{i\alpha}^s da_\alpha^s, \quad (5.10)$$

determined by a generally nonsymmetric tensor defined at each sampling point.

(3) Being a result of local thermodynamic processes, the instantaneous rate of change $\dot{da}_\alpha^s$ of a line element da_α^s in the configuration of $\mathcal{N}^s$ in the natural reference state with respect to itself is given by the linear mapping relation,

$$\dot{da}_\alpha^s = {}^i\Lambda_{\alpha\beta}^s da_\beta^s, \quad (5.11)$$

with ${}^i\Lambda_{\alpha\beta}^s$ a generally nonsymmetric tensor defined at each sampling point.

With s^s denoting the entropy per unit mass in sampling point s , the thermodynamic state of

a finite element of a material possessing a natural reference state is assumed to be characterized completely by the vectors $s = [s^s]^t$ and $c_{i\alpha} = [c_{i\alpha}^s]^t$, $s = 1, \dots, s^e$. According to the deterministic approach adopted by Van der Giessen [5], given nodal velocities v_i along with given nodal entropy fluxes h_i and a given thermodynamic state $\{s, c_{i\alpha}\}$, $i, \alpha = 1, \dots, p$, shall completely determine the subsequent motion of the element and the accompanying internal processes.

5.4. A variational approach

For the derivation of the finite element analogues of the field equations of thermomechanics, a variational formulation encompassing these equations is most appropriate. In a series of papers, Biot has developed a variational approach to irreversible thermodynamics similar to the Lagrangian approach in classical mechanics [4]. It is a comprehensive approach which, from a single variational statement, not only provides the governing field equations, but also the additional constitutive equations. This latter however requires a particular type of constitution of the material under consideration. In this section we shall apply Biot's approach to the present discrete model, confining ourselves in doing so to the (discrete analogues of the) thermomechanical field equations for materials possessing a natural reference state. Constitutive equations, in particular for the irreversible processes, will be discussed in Section 6.

Let us consider an element in some thermomechanical state characterized by $\{v_i, h_i, s, c_{i\alpha}\}$. Following Biot [4], now consider variations described by vectors δu_i and δh_i of virtual nodal displacements and entropy displacements, respectively. Notice that we only apply variations of external variables.

In the field description, the material rates of change of mass density and entropy accompanying the flow of mass and of entropy, described by the fields v_i and h_i , are governed by

$$\dot{\rho} = -\rho \frac{\partial v_k}{\partial x_k}, \quad \rho \dot{s} = -\frac{\partial \dot{h}_k}{\partial x_k} + \rho \dot{\sigma}, \quad (5.12)$$

where $\dot{\sigma}$ is the rate of entropy production per unit mass. In the present finite element formulation, the discrete equivalents of these balance equations for each element are again obtained by local application of (5.12); this leads to

$$\dot{\rho} = -\rho D_k v_k, \quad \rho \dot{s} = -D_k \dot{h}_k + \rho \dot{\sigma}, \quad (5.13)$$

with D_k the matrix also entering (5.7) and given by (5.8) for the quadratic spatial element, and $\dot{\sigma}$ the vector of entropy production rates at the sampling points, $\dot{\sigma} = [\dot{\sigma}^s]^t$, $s = 1, \dots, s^e$. The material rates $\dot{\rho}$ and $\dot{s}$ in a spatial description follow from (5.2). Since $\sum_s \rho^s V^s$ is the mass of the element, it follows from (5.13) that the material rate of change of the vector of sampling point volume fractions, $V = [V^s]^t$ is given by,

$$\dot{V} = V D_k v_k.$$

Similarly the virtual (entropy) displacements induce variations $\delta \rho$ and δs of the mass

density, volume fraction, and entropy at the sampling points according to

$$\delta \rho = -\rho D_k \delta u_k, \quad \delta V = V D_k \delta u_k, \quad \rho \delta s = -D_k \delta h_k + \rho \delta \sigma, \quad (5.14)$$

where $\delta \sigma$ is the vector of the sampling point variations in the entropy produced in the given state due to the virtual entropy displacements. Very much like Biot [4] and in the spirit of the present approach, we shall assume that the variation $\delta \sigma^s$ at any sampling point s is related to the local virtual entropy displacement δh_i^s according to,

$$\rho \delta \sigma = N_i \delta H_i, \quad (5.15)$$

where $\delta H_i = [\delta h_i^s]^t$, $s = 1, \dots, s^e$, is evaluated by interpolation between the nodal virtual entropy displacements,

$$\delta H_i := B \delta h_i \quad (5.16)$$

(cf. (5.3)). $N_i = [N_i^s]^t$ is the vector of entropy production forces at the sampling points, which are determined by the constitution (see Section 6).

Following Biot [4] it is now asserted that for each finite element in a given thermomechanical state, the following *virtual energy balance* is to be satisfied,

$$\delta U = \delta W + \delta Q, \quad (5.17)$$

for all virtual displacements δu_i and all virtual entropy displacements δh_i . Here, U is the internal energy of the finite element, δW is the virtual work, and δQ is the virtual heat supplied to the element by its surrounding elements at virtual entropy displacements δh_i . With u^s denoting the internal energy per unit mass at sampling point s , U is evaluated by the weighted sum of the internal energy at the element sampling points,

$$U = \sum_{s=1}^{s^e} \rho^s u^s V^s,$$

similar to $U = \int \rho u dV$ in the field description.

The virtual work δW comprises of (i) the virtual work δW^e of the external forces acting at the element boundary due to the interactions with the surrounding elements and (ii) the virtual work δW^i of the internal (body) forces, including according to d'Alembert's principle, the virtual work of the reversed inertia forces. The body forces (e.g., due to gravity) and the inertia forces are forces acting on the material contained within the element. It is in the spirit of the sampling point approach, then, to sample the virtual work of these forces in the material sampling points. For the internal virtual work δW^i we therefore write,

$$\delta W^i = \sum_{s=1}^{s^e} \rho^s V^s (f_i^s - \dot{v}_i^s) \delta u_i^s = [\rho V (f_i - \dot{V}_i)]^t \delta U_i, \quad (5.18)$$

with f_i , $\dot{V}_i$, and δU_i the vectors of the body forces per unit mass, the material acceleration, and

the virtual displacements, respectively, at the sampling points. The latter two are given by interpolation between the nodal accelerations and virtual displacements (cf. (5.3) and (5.16)):

$$\dot{V}_i := B \dot{v}_i, \quad \delta U_i := B \delta u_i. \quad (5.19)$$

Similar to the approach put forward in Section 5.1, the material accelerations $\dot{v}_i$ at the nodal points are evaluated from

$$\dot{v}_i = \frac{\partial v_i}{\partial t} + v_k \Delta_k v_i,$$

where Δ_k is the $n^e \times n^e$ matrix of the gradients of the interpolation functions for the nodal quantities at the nodal points. For the two-dimensional quadratic element, we find from (3.2),

$$2A \Delta_i = \begin{bmatrix} 3g_i^1 & -g_i^2 & -g_i^3 & 4g_i^2 & 0 & 4g_i^3 \\ -g_i^1 & 3g_i^2 & -g_i^3 & 4g_i^1 & 4g_i^3 & 0 \\ -g_i^1 & -g_i^2 & 3g_i^3 & 0 & 4g_i^2 & 4g_i^1 \\ g_i^1 & g_i^2 & -g_i^3 & 2(g_i^1 + g_i^2) & 2g_i^3 & 2g_i^3 \\ -g_i^1 & g_i^2 & g_i^3 & 2g_i^1 & 2(g_i^2 + g_i^3) & 2g_i^1 \\ g_i^1 & -g_i^2 & g_i^3 & 2g_i^2 & 2g_i^2 & 2(g_i^3 + g_i^1) \end{bmatrix}$$

Referring to (3.1), the external virtual work and the virtual heat are given by

$$\delta W^e = t_i^t \delta u_i, \quad \delta Q = -T_i^t \delta h_i. \quad (5.20)$$

Let us now consider the consequences of this variational statement for a continuous medium to which a natural reference state can be attributed. According to the theory of the natural reference state [5] the internal energy u^s at a sampling point s is at any instant completely determined by the instantaneous local values of s^s and the strain tensor $E_{\alpha\beta}^s$ with respect to the natural reference geometry defined by,

$$E_{\alpha\beta}^s = \frac{1}{2}(c_{i\alpha}^s c_{i\beta}^s - \delta_{\alpha\beta}).$$

With the internal energy function,

$$u^s = u^s(s^s, E_{\alpha\beta}^s),$$

the variation of the internal energy of the element becomes,

$$\delta U = \sum_{s=1}^{s^e} \rho^s V^s \left(\frac{\partial u^s}{\partial s^s} \delta s^s + \frac{\partial u^s}{\partial E_{\alpha\beta}^s} \delta E_{\alpha\beta}^s \right). \quad (5.21)$$

Notice that the variation of $\rho^s V^s$ vanishes by virtue of (5.14a), (5.14b). With the aid of (5.14a)

and (5.15), (5.16), δs^s can be expressed in terms of $\delta \mathbf{h}_i$ immediately. In order to express $\delta E_{\alpha\beta}^s$ in terms of $\delta \mathbf{u}_i$, we first derive from (5.10) and $\delta \mathbf{d}\mathbf{x}_i = (D_j \delta \mathbf{u}_i) \mathbf{d}\mathbf{x}_j$, similar to (5.6), (5.7),

$$\delta \mathbf{c}_{i\alpha} = (D_j \delta \mathbf{u}_i) \mathbf{c}_{j\alpha} , \quad (5.22)$$

since the geometry in the natural reference state, as characterized by $d\mathbf{a}_\alpha^s$, remains unaffected by virtual displacements by definition. With the aid of (5.22), $\delta E_{\alpha\beta}^s$ may be expressed as,

$$\delta E_{\alpha\beta}^s = c_{i\alpha}^s \delta \varepsilon_{ij}^s c_{j\beta}^s ,$$

with $\delta \varepsilon_{ij}^s$ the virtual strain tensor induced by the virtual displacements and which for each element, $\delta \boldsymbol{\varepsilon}_{ij} = [\delta \varepsilon_{ij}^s]^t$, is defined by,

$$\delta \boldsymbol{\varepsilon}_{ij} = \frac{1}{2} (D_i \delta \mathbf{u}_j + D_j \delta \mathbf{u}_i) , \quad (5.23)$$

similar to the expression (5.9a) for the vector of actual strain rates $\mathbf{D}_{ij}$. Then the expression for the variation of the internal energy of an element, (5.21), can be rewritten as,

$$\delta U = \sum_{s=1}^{s^e} V^s (\theta^s \rho^s \delta s^s + \sigma_{ij}^s \delta \varepsilon_{ij}^s) = (\mathbf{V}\boldsymbol{\theta})^t \boldsymbol{\rho} \delta \mathbf{s} + (\mathbf{V}\boldsymbol{\sigma}_{ij})^t \delta \boldsymbol{\varepsilon}_{ij} , \quad (5.24)$$

with $\boldsymbol{\theta} = [\theta^s]^t$ and $\boldsymbol{\sigma}_{ij} = [\sigma_{ij}^s]^t$, $s = 1, \dots, s^e$, where θ^s and σ_{ij}^s are defined by,

$$\theta^s := \frac{\partial u^s}{\partial s^s} , \quad \sigma_{ij}^s := \rho^s c_{i\alpha}^s \frac{\partial u^s}{\partial E_{\alpha\beta}^s} c_{j\beta}^s , \quad (5.25)$$

and may be interpreted as the *temperature* and the (symmetric) *stress tensor* at sampling point s , respectively. It is emphasized that these quantities are determined by the local thermodynamic state through the locally defined internal energy function.

Substituting (5.14c) and (5.15) into (5.24) to eliminate δs , and invoking (5.18) and (5.20), the virtual energy balance (5.17) reads,

$$\begin{aligned} & (\mathbf{V}\boldsymbol{\sigma}_{ij})^t \delta \boldsymbol{\varepsilon}_{ij} - [\boldsymbol{\rho} \mathbf{V}(f_i - \dot{V}_i)]^t \delta U_i - (\mathbf{V}\boldsymbol{\theta})^t D_k \delta \mathbf{h}_k + (\mathbf{V}\boldsymbol{\theta} N_i)^t \delta H_i \\ & = \mathbf{t}_i^t \delta \mathbf{u}_i - \mathbf{T}_i^t \delta \mathbf{h}_i \quad \forall \delta \mathbf{u}_i, \delta \mathbf{h}_i . \end{aligned}$$

With the aid of (5.16), (5.19), and (5.23), this condition then provides for each element the *discrete equations of motion*,

$$D_j^t \mathbf{V}\boldsymbol{\sigma}_{ij} - B^t \boldsymbol{\rho} \mathbf{V}(f_i - \dot{V}_i) = \mathbf{t}_i , \quad (5.26)$$

and the *discrete heat flow equations*,

$$D_i^t \mathbf{V}\boldsymbol{\theta} - B^t \mathbf{V}\boldsymbol{\theta} N_i = \mathbf{T}_i . \quad (5.27)$$

The equations (5.13) and (5.26), (5.27) constitute the discrete analogues for each element of

the differential balance equations of thermomechanics in the field description. The finite element equations for the entire model may be compiled in the usual way.

By virtue of the fact that δu_i and δh_i are independent, the virtual energy balance (5.17) combines the virtual work and the virtual heat equations used separately by Besseling [3]. In an approach based upon the principles of virtual work and virtual heat [3], stress and temperature are introduced as multipliers for which the constitutive equations are to be formulated subsequently, whereas in this approach they appear as quantities defined by the thermodynamic state through (5.25) (cf. also [1]). Which one of these viewpoints is preferred over the other seems just a matter of taste.

6. Constitutive equations

The general discrete balance equations derived in the previous section are to be completed by adding the constitutive equations for the sampling point quantities in terms of locally defined state variables and the local material properties (in an inhomogeneous medium). In formulating these equations it should be observed that as a consequence of the sampling point approach, *any constitutive theory* formulated within the framework of the natural reference state in terms of the continuum model, e.g. [1, 5, 6], *can immediately be applied locally at the sampling points*. In addition to the elegance of such an approach, it adds to the simplicity of the formulation of the final set of equations particularly in the case of complex, nonlinear material behaviour (of inhomogeneous materials).

With known internal energy functions u^s at all sampling points, the stresses σ_{ij}^s and temperature θ^s are given by the expressions (5.25). Next, constitutive equations are needed for the entropy production forces N_i^s and the rates of deformation $\dot{\Lambda}_{\alpha\beta}^s$ due to the irreversible deformation processes (cf. (5.11)). Since the constitutive equations for the latter quantities strongly depend on the type of material under consideration, we shall not go into the subject here; suffice it to refer the reader to e.g. [1, 5, 6].

Let us briefly discuss the constitutive equations for the vector of entropy production forces $N_i = [N_i^s]^t$, $s = 1, \dots, s^e$, in the heat flow equations (5.27). Due to the actual entropy fluxes $\dot{h}_i$, these forces give rise to an entropy production rate per unit volume at the sampling points according to

$$\rho \dot{\sigma} = N_i \dot{H}_i, \quad (6.1)$$

similar to (5.15), with $\dot{H}_i = [\dot{h}_i^s]^t$ the vector of entropy fluxes at the element sampling points (cf. (5.16)):

$$\dot{H}_i = B \dot{h}_i.$$

The energy dissipation rate at a sampling point s due to the entropy flow process is thus given by the expression

$$\mathcal{D}^s = \rho^s \theta^s \dot{\sigma}^s = \theta^s N_i^s \dot{h}_i^s \geq 0,$$

and is assumed to be completely determined by the instantaneous local state.

Following the constitutive theory for materials possessing a natural reference state [5], we introduce at each sampling point a dissipation function,

$$\Phi^s = \theta^s \eta^s \left(\theta^s, \frac{\rho_0^s}{\rho^s} c_{\alpha i}^{s-1} \dot{h}_i^s \right) \geq 0,$$

such that $N_i^s \dot{h}_i^s = \eta^s$ and we define the thermodynamic force N_i^s through the orthogonality condition,

$$N_i^s = \nu^s \frac{\partial \eta^s}{\partial \dot{h}_i^s}, \quad \nu^s = \left(\frac{\partial \eta^s}{\partial \dot{h}_i^s} \dot{h}_i^s \right)^{-1} \eta^s.$$

The factor $\rho_0^s / \rho^s c_{\alpha i}^{s-1}$ in the entropy flux dependence of Φ^s , ρ_0^s being the mass density in the natural reference state, is typical for the constitutive theory of the natural reference state and accounts for the influence of the elastic deformations on the actual heat conductivities [5]. Neglecting such effects as well as the influence of temperature, a suitable expression for η^s reads

$$\eta^s = \dot{h}_i^s k_{ij}^{s-1} \dot{h}_j^s, \quad (6.2)$$

where k_{ij}^{s-1} are positive-definite material constants which can be interpreted as the inverse local heat conductivity coefficients. In the case of a homogeneous isotropic material for instance, we have $k_{ij}^s = k$ for all sampling points and the vector N_i is simply given by,

$$N_i = k^{-1} \dot{H}_i.$$

Finally we note that for instance elastoplastic and viscoelastic materials are governed by rate constitutive equations for the stresses in terms of the continuum deformation. The rate equilibrium equations required in a quasistatic finite element analysis of such materials may be obtained by straightforward (material or spatial) differentiation of the equilibrium equations $D_j^t V \sigma_{ij} = t_i$ (from (5.26)).

7. Examples

7.1. A two-dimensional linear elasticity problem

As a simple example of two-dimensional thermomechanical processes, let us briefly consider the classical problem of small isothermal, quasistatic deformations of a homogeneous, isotropic, linearly elastic body. With a quadratic expression for the internal energy function at any sampling point in terms of the local elastic strains, the sampling point stresses are according to (5.25b) given by,

$$\sigma_{ij}^s = (C - \frac{2}{3}G) E_{kk}^s \delta_{ij} + 2G E_{ij}^s,$$

with C the compression modulus, G the shear modulus, and E_{ij}^s the components of the elastic strain tensor with respect to the global frame of reference.

We now note that in the case of isothermal deformations of a purely elastic body, the finite element theory presented here reduces to one which is basically equivalent with that proposed by Besseling [2]. In fact a linear elastic analysis of the in-plane deformations of a square plate loaded in bending and shear, employing the quadratic two-dimensional element discussed here (Fig. 2), has been carried out by Besseling [2]. For a 12×6 triangular mesh for half the plate, results were found for the displacements and stresses that have the same accuracy as results obtained with the traditional method [9].

7.2. A one-dimensional heat conduction problem

With regard to heat flow processes, it should be observed that in the present approach the accompanying entropy production in a finite element is evaluated as a weighted sum of the entropy productions sampled at the sampling points. This is in contrast with more traditional methods in which the entropy production in an element would typically be evaluated from an integral over the element (cf. e.g. [3]). The differences in approach find expression for instance in the second term, associated with entropy production, on the left-hand side of the heat flow equation (5.27). In order to gain some insight into the accuracy obtained with our approach, in particular in the case of considerable temperature gradients, we shall briefly consider a simple one-dimensional heat conduction problem.

A wall of constant thickness l is completely insulated at one side, while the other from $t = 0$ is exposed to a temperature increased by a constant ΔT_0 with respect to the previous uniform temperature T_0 . The wall is modelled by two quadratic, one-dimensional elements each containing

$$n^e = \binom{3}{2} = 3$$

nodal points and

$$s^e = \binom{2}{1} = 2$$

material sampling points (see Fig. 3). Application of the conditions discussed in Section 4—in much the same way as for the two-dimensional element—yields that the sampling points within each element should be positioned on each side of the center at a distance $\frac{1}{3}\sqrt{3}L$ ($2L$ being the element length).

Assuming small entropy changes associated with the temperature changes, we may use a quadratic expression for u^s in terms of s^s and, from (5.25a), we find the sampling point temperatures to be given by,

$$\theta^s = T_0(1 + s^s/c_v), \quad (7.1)$$

with c_v the specific heat per unit mass. Together with (7.1), the problem is governed by (5.27), (5.13b), and (6.1), (6.2). The problem may be linearized by observing that the influence of the entropy production on the temperature through (7.1) may be neglected, provided that the temperature changes remain small as compared with T_0 [3]. The boundary

Fig. 3. One-dimensional heat conduction problem.

conditions to be applied read $\dot{h}^5 \equiv 0$ and $T^1 = -T$ (since $\dot{Q} = Th^1$ is the rate of heat supply through the boundary $x = 0$, see (3.1b)).

Figure 3 shows the solution of the linearized problem in comparison with the exact solution of the continuum problem and the finite element solution of Besseling [3]. It is observed that the results obtained with the present method are definitely not worse than those obtained by Besseling. Despite the use of two elements only, the average temperature distribution is approximated well.

8. Conclusion

Without going into any detail, it will be evident that the concept of material sampling points is somehow related to that of the commonly used Gaussian integration points [9]. On the other hand, however, these concepts should be clearly discriminated from one another since they are fundamentally different in nature: the latter are purely mathematical entities introduced in connection with the evaluation of the often complicated element matrices encountered in Galerkin type methods, whereas material sampling points are in fact considered here as *basic physical concepts in the thermomechanics of finite elements*. The number of sampling points and their position within an element follow from well-founded physical arguments, rather than from accuracy and convergence considerations.

Employing the notion of material sampling points, we have obtained a *complete discrete analogue of continuum theory*. The role of the material points in the continuum theory is taken

over in the finite element theory by that of material sampling points. The physical quantities involved are represented by finite-dimensional vectors rather than by continuous fields, while the differential equations and associated boundary conditions are replaced with finite sets of fully algebraic equations. The set of physical quantities breaks up into the set of quantities defined at the nodal points which represent the spatial interactions between elements and the set of quantities defined at the material sampling points which characterize the state of the material.

In addition to its elegance the present finite element theory has the computational advantages over traditional methods that the final equations involve no integrals at all. This will result in a substantial reduction of computational effort, particularly in physically nonlinear problems, since extensive numerical integration is no longer needed.

The finite element theory presented here allows for a spatial formulation for flow problems as well as for a material formulation for deformation problems. Within the framework of the theory of the natural reference state, nonlinear constitutive models are included for a wide range of materials from gases to highly deformable elastoplastic solids, while even more complicated models (for elastoplasticity e.g.) are currently being developed.

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