A thermomechanical formulation of finite element schemes for micropolar continua

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Abstract

Recent studies highlighted the advantages of the thermomechanical approach for developing models of material behaviour. This approach ensures compliance with thermodynamical laws since constitutive relations are derived from a consideration of thermodynamical potentials. Interestingly, the same thermomechanical techniques can also be used to formulate the finite element models used to implement these constitutive relations. Thus the key advantage of this type of finite element formulation is that a direct link to the underlying physics of the problem is extended through to the model's implementation. Here, we show how the thermomechanical approach can be applied to finite element schemes for models based on micropolar continuum theory.

[0]This paper is dedicated to Professor Jim Hill on the occasion of his 60th birthday.

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Material points that make up a micropolar continuum possess rotational degrees of freedom, in addition to the conventional translational degrees of freedom. Hence, the equations governing boundary value problems for this class of materials differ from those of their classical counterparts—both from the viewpoint of the constitutive law and the governing conservation laws. We outline the development of finite element schemes for elastic and plastic micropolar materials using the thermomechanical approach. The analysis indicates that while the traditional Galerkin method admits a range of weighting functions, the second law of thermodynamics provides an additional constraint that narrows the choice of admissible functions.

Contents

1 Introduction

A material point in a classical continuum has three translational degrees of freedom. While this type of continuum is appropriate for most materials, there are a number of materials that are better represented as continua with

additional degrees of freedom: for example, fibrous composites (Lakes [6]), granular materials (Tordesillas and Walsh [10]), and some biological materials like bone (Onck [8]). In cases where a material is composed of relatively rigid micro-scale structures that can spin independently, a micropolar or Cosserat continuum might be more appropriate. Unlike a classical continuum, the motion of each point in a micropolar continuum is described both by a displacement and a rotation.

Whether based on micropolar or classical continua, all constitutive models must obey the laws of thermodynamics. However, in most cases this basic requirement is enforced retroactively, that is, constitutive laws are first proposed and thermodynamical restrictions are then applied as a constraint. There are two disadvantages to this approach:

- the added constraints may unduly limit the model's behaviour;
- the constraints may not restrict the model adequately, leading to non-physical results.

Alternatively, a thermomechanical approach can be used to develop the model. This approach was first developed for classical materials as a means of ensuring physical behaviour without introducing unnecessary restrictions into the model (Ziegler [14], Collins and Houlsby [2]). The material behaviour is first described in terms of two thermodynamical potentials. Constitutive relations and the underlying balance equations are then derived directly from the first and second laws of thermodynamics using these potentials. Walsh and Tordesillas [13] recently demonstrated the use of this approach in the development of micropolar constitutive models of granular media. For further details on the application of the modern theory of thermomechanics to constitutive modelling, see [13] and the papers cited therein.

An important advantage of the thermomechanical approach is that it need not be limited to the development of constitutive laws alone. The same

ideas can be applied in the formulation of finite element schemes. While this type of approach is common practice in the development of elastic finite element models (FEMs), the same cannot be said for plastic materials. Many models of plastic behaviour are based on quasi-thermodynamic postulates rather than the laws of thermodynamics themselves (Lubliner [7]). Thus it can be difficult to relate the model's numerical implementation to the physics underlying the material behaviour. In contrast, a thermomechanical formulation of the finite element scheme establishes this link from the outset.

Here we discuss how a thermomechanical approach is applied to the formulation of finite element models of micropolar materials. Section 2 outlines the theory behind micropolar continua. In Section 3 we show how finite element schemes are derived for elastic and plastic materials using the thermomechanical formulation. Conclusions are drawn in Section 4.

2 Micropolar continuum

The motion of a point in a classical continuum is described by a single displacement vector u_i. Any rotation experienced by the point is due to gradients in the displacement field. In contrast, points within a micropolar continuum may experience rotations which are independent of the displacement field. Accordingly, each point is assigned a rotation vector ω_i. The rotation vector may be decomposed into two parts: a gross body rotation, Γ_i, describing rotation due to the point's motion about an external reference frame; plus an additional component due to the point's intrinsic spin, ψ_i. The gross body rotation is related to the vector field via

$$\Gamma_i = -\frac{1}{2} e_{ijk} u_{j,k} \,, \tag{1}$$

where e_{ijk} is the permutation tensor ($e_{123} = e_{231} = e_{312} = -e_{213} = -e_{132} = -e_{321} = 1$), and subscript commas imply differentiation, that is, $()_{,i} = \partial()/\partial x_i$.

The deformation of a micropolar continuum is described by two tensor quantities: the microstrain ϵ_{ij} and the curvature κ_{ij}. The microstrain and curvature are related to the displacement and rotation fields by

$$\epsilon_{ij} = u_{i,j} + e_{ijk}\omega_k \,, \tag{2}$$
$$\kappa_{ij} = \omega_{i,j} \,. \tag{3}$$

Individual points in a micropolar continuum transmit moments as well as forces, giving rise to a stress-like tensor known as the couple stress. Just as the force f_i per unit area of a surface with a unit normal vector n_i is related to the stress σ_{ij} via

$$f_i = \sigma_{ij} n_j \,, \tag{4}$$

the moment per unit area m_i is related to the couple stress μ_{ij} via

$$m_i = \mu_{ij} n_j \,. \tag{5}$$

The equations of equilibrium governing the stress and couple stress are

$$\sigma_{ij,j} = 0 \,, \tag{6}$$
$$\mu_{ij,j} - e_{ijk}\sigma_{jk} = 0 \,. \tag{7}$$

Note that the stress tensor is no longer symmetric. The anti-symmetric component is needed to balance additional moments created by the couple stress.

Stress-strain relations for micropolar continua can be developed using a thermomechanical approach (Walsh and Tordesillas [13]). In the thermomechancial approach, the constitutive model is developed based on a consideration of two potential functions. Here we use the free energy ψ and the dissipation function D, although other combinations of energy functions are possible (Collins and Houlsby [2]). Equations relating the potential functions to the kinematic variables can be obtained from the first and second laws of

thermodynamics. It may be shown that the following equations hold for the free energy and the dissipation function:

$$\sigma_{ij} - \frac{\partial \psi}{\partial \epsilon_{ij}} = 0\,, \quad \mu_{ij} - \frac{\partial \psi}{\partial \kappa_{ij}} = 0\,, \quad \mu_{ij,j} - \frac{\partial \psi}{\partial \omega_i} = 0\,, \tag{8}$$

$$\frac{\partial \psi}{\partial \epsilon^p_{ij}} + \frac{\partial D}{\partial \dot{\epsilon}^p_{ij}} = 0\,, \quad \frac{\partial \psi}{\partial \kappa^p_{ij}} + \frac{\partial D}{\partial \dot{\kappa}^p_{ij}} = 0\,, \tag{9}$$

where ϵ^p_{ij} is the plastic strain and κ^p_{ij} is the plastic curvature. Stress-strain relations for specific materials are derived from these equations by expressing the free energy and dissipation function in terms of the strain and curvature.

3 Thermomechanical finite element formulation

The discussion that follows is divided into two subsections. The first outlines the formulation of finite element models for elastic micropolar materials, while the second provides an outline of the theory for micropolar materials undergoing plastic deformation. In both subsections a "thermomechanical" approach is taken in which the equations governing the finite elements are determined from a consideration of the thermodynamics of the material body. Houlsby and Puzrin [5] give an example of the thermomechanical approach applied to classical FEM.

Although the theory is applicable to three dimensional models, for the sake of brevity and simplicity, the examples given in the discussion refer to two dimensional models alone.

3.1 Elastic micropolar models

The finite element method approximates the behaviour of a continuum by subdividing the body into a finite number of regions or elements. Each element is connected to its neighbours through a set of points or nodes. Constitutive variables describing the state of the material body are assigned to each node. The values of the constitutive variables within each element are assumed to be simple functions of these nodal values. For example, the displacements and rotations within each element are related to the nodal displacements and rotations by interpolation functions, that is,

$$\{u\} = [N]\{d\}\,, \tag{10}$$

where $\{u\}$ is a vector made up of the displacement and rotation field components, $[N]$ is the interpolation function matrix and $\{d\}$ is a vector composed of the displacements and rotations of the nodal points. A convention of combining displacement and rotation components into a single vector is used throughout this paper. For example, in two dimensions, the vector

$$\{u\} = \left\{ \begin{array}{c} u_1 \\ u_2 \\ \omega \end{array} \right\}\,, \tag{11}$$

where u_i are the components of the displacement field within the element and ω is the rotation field within the element. This has been done for the sake of brevity and to highlight similarities with conventional finite element methods.

Once the continuum has been subdivided, the problem becomes one of finding the nodal displacements for a given set of boundary conditions. A relationship between the nodal points' displacements and the applied forces are found using thermodynamical principles. For an elastic material, the first law of thermodynamics states that a variation in the internal energy of each element, δU_e, is equal to the external work done on the nodes, δW_e, that is,

$$\delta U_e = \delta W_e\,. \tag{12}$$

The external work is the product of the vector of external forces and moments acting on the nodes, $\{f\}$, with the respective virtual nodal displacements and rotations, $\{\delta d\}$:

$$\delta W_e = \{\delta d\}^T \{f\} \,. \tag{13}$$

The internal energy

$$\delta U_e = \int_V \{\delta\epsilon\}^T \{\sigma\} \, dV \,, \tag{14}$$

where V is the volume (or area in two dimensions) of the element, $\{\delta\epsilon\}$ is a vector composed of the virtual strain and curvature components arising from the virtual nodal displacements, and the vector $\{\sigma\}$ contains the stress and couple stress components. The stress and strain vectors are

$$\{\sigma\} = \{\sigma_{11} \,,\, \sigma_{22} \,,\, \sigma_{12} \,,\, \sigma_{21} \,,\, \mu_1 \,,\, \mu_2\}^T \,, \tag{15}$$

$$\{\epsilon\} = \{\epsilon_{11} \,,\, \epsilon_{22} \,,\, \epsilon_{12} \,,\, \epsilon_{21} \,,\, \kappa_1 \,,\, \kappa_2\}^T \,. \tag{16}$$

The strain and curvature components $\{\epsilon\}$ are obtained from the nodal displacements $\{d\}$ using an element matrix $[B]$ such that

$$\{\epsilon\} = [B]\{d\} \,. \tag{17}$$

The strain-displacement matrix, $[B]$, is found in turn using the expression for the displacement and rotation field components in equation (10). From the definition of the strain and the curvature in equation (2) and equation (3), the matrix

$$[B] = [\partial^*][N] \,, \tag{18}$$

where the operator

$$[\partial^*] = \begin{bmatrix} \frac{\partial}{\partial x} & 0 & 0 \\ 0 & \frac{\partial}{\partial y} & 0 \\ \frac{\partial}{\partial y} & 0 & 1 \\ 0 & \frac{\partial}{\partial x} & -1 \\ 0 & 0 & \frac{\partial}{\partial x} \\ 0 & 0 & \frac{\partial}{\partial y} \end{bmatrix} \,. \tag{19}$$

Unlike the classical case, this matrix is not only made up of partial derivatives of the interpolation functions but also the functions themselves.

For a linear elastic material the stress and couple stress components are related by

$$\{\sigma\} = [E]\{\epsilon\}\,, \tag{20}$$

where $[E]$ is the elastic stiffness matrix. Using this identity and the virtual work equation (12) we have

$$[K_e]\{d\} = \{f\}\,, \tag{21}$$

where the element stiffness matrix

$$[K_e] = \int_V [B]^T[E][B]\,dV\,. \tag{22}$$

Whereas the derivation of the stiffness matrix is similar to that of a classical continuum element, differences do exist in the details of the computation. To highlight the differences between the FEM formulation for classical and micropolar continua, let us turn our attention to the calculation of the stiffness matrix for a two dimensional element. To simplify the discussion, we consider the behaviour of a linear triangular element.

For a triangular element with three nodes, the shape function $[N]$ is a linear function of position. For classical materials, this means that the strain-displacement matrix $[B]$ (and hence the integrand in the element stiffness matrix) is constant throughout the element. However, in the micropolar case, the integrand in the element stiffness matrix varies within the element. The integrand for the micropolar material can be either evaluated directly or using Gauss quadrature. Either way, the computation for the integrand results in a significant increase in the amount of CPU time required to calculate the element stiffness matrix.

The varying integrand in the element stiffness matrix arises because the rotation field is given by a polynomial of the same order as that used in

the element's displacement field. One might be tempted to reduce the order of the rotation polynomial used in order to speed up the calculation. For a linear triangular element however, this would result in a classical model as constant rotation gives zero curvature within the element. In elements with more nodes (and hence higher orders of interpolation) this step may be justified (Ehlers and Volk [4]).

We stress that even when using higher order elements, numerical quadrature rules used for classical continua do not necessarily translate automatically to micropolar finite element methods. For example, in a classical framework, 2×2 quadrature rules are sufficient to obtain a convergent solution when using eight-node quadrilateral elements. However, this is not true of micropolar finite elements, which need 3×3 quadrature points to ensure convergence for quadratic interpolation (Adhikary and Dyskin [1]).

3.2 Plastic micropolar models

For plastic materials, the first law of thermodynamics is

$$\delta\psi_e = \delta W_e - D_e \,, \tag{23}$$

where $\delta\psi_e$ is a variation in the free energy and D_e is the rate of dissipation of the element. Equation (23) is rewritten as

$$\int_V \{\delta\epsilon\}^T \left\{\frac{\partial\psi}{\partial\epsilon}\right\} dV = \{\delta d^t\}^T\{f\} - \int_V \{\delta\epsilon^P\}^T\{\chi\}\, dV \,, \tag{24}$$

where $\{\chi\}$ are the dissipative stresses and couple stresses; and $\{\epsilon^P\}$ are the plastic strains and curvatures. Here the strain vector $\{\epsilon\}$ is composed of both the total strain and plastic strain components:

$$\{\epsilon\} = \left\{\epsilon^t_{11}\,,\ \epsilon^t_{22}\,,\ \epsilon^t_{12}\,,\ \epsilon^t_{21}\,,\ \kappa^t_1\,,\ \kappa^t_2\,,\ \epsilon^p_{11}\,,\ \epsilon^p_{22}\,,\ \epsilon^p_{12}\,,\ \epsilon^p_{21}\,,\ \kappa^p_1\,,\ \kappa^p_2\right\}^T \,. \tag{25}$$

Likewise, the vector $\{d\}$ contains new variables in addition to the nodal points' rotations and displacements. The components of the plastic strains and curvatures are written in terms of plastic displacements u_i^p and rotations ω^p:

$$\epsilon_{ij}^p = u_{i,j}^p + e_{ij3}\omega^p \,, \tag{26}$$

$$\kappa_i^p = \omega_{,i}^p \,. \tag{27}$$

Like the displacement and rotation variables, the values of the plastic displacement and rotation variables within each element are determined by interpolating the values of the variables at the node points d^p, that is,

$$\{u^p\} = [N]\{d^p\} \,. \tag{28}$$

The second law of thermodynamics is satisfied by requiring that the rate of dissipation is non-negative:

$$D_e = \{\delta d^p\}^T \int_V [B]^T \{\chi\}\, dV \geq 0 \,. \tag{29}$$

Expressing equation (24) in terms of the nodal displacements gives

$$\{\delta d\}^T \int_V [B]^T \left\{\frac{\partial \psi}{\partial \epsilon}\right\} dV = \{\delta d^t\}^T \{f\} - \{\delta d^p\}^T \int_V [B]^T \{\chi\}\, dV \,. \tag{30}$$

This equation must hold for all arbitrary variations in the nodal displacements $\{\delta d\}$, and consequently may be decomposed into two parts, representing contributions from the total strain and plastic strain components:

$$\int_V [B]^T \left\{\frac{\partial \psi}{\partial \epsilon^t}\right\} dV = \{f^t\} \,, \tag{31}$$

$$\int_V [B]^T \left\{\frac{\partial \psi}{\partial \epsilon^p}\right\} dV = -\int_V [B]^T \{\chi\}\, dV \,, \tag{32}$$

where equation (32) holds if $\int_V \|\{\delta\epsilon^p\}\|\, dV \neq 0$. Note that this step is not as trivial as it would first appear due to the dependence of $\{\chi\}$ on the increment

in the plastic strain. For a more detailed discussion we refer the reader to Valanis [12] and Walsh and Tordesillas [13].

The finite element equations derived using the thermomechanical approach are equivalent to those obtained via the Galerkin formulation. Using this formulation, the equations of equilibrium are rewritten as a set of weighted integrals:

$$\int_V [W]^T \sigma_{ij,j}\, dV = 0\,; \quad \int_V [W]^T (\mu_{i,i} - e_{ij3}\sigma_{ij})\, dV = 0\,; \tag{33}$$

$$\int_V [W]^T \left(\frac{\partial \psi}{\partial \epsilon^p_{ij}} + \frac{\partial D}{\partial \dot{\epsilon}^p_{ij}} \right) dV = 0\,; \quad \int_V [W]^T \left(\frac{\partial \psi}{\partial \kappa^p_{ij}} + \frac{\partial D}{\partial \dot{\kappa}^p_{ij}} \right) dV = 0\,. \tag{34}$$

Setting the weighting function $[W]^T = [N]^T$ in (33) and integrating by parts gives

$$\int_S [N]^T \sigma_{ij} n_j dS = \int_V [N]^T_{,j} \sigma_{ij}\, dV\,, \tag{35}$$

$$\int_S [N]^T \mu_i n_i dS = \int_V ([N]^T e_{ij3}\sigma_{ij} + [N]^T_{,i}\mu_i)\, dV\,, \tag{36}$$

which is equivalent to equation (31). Similarly, equation (32) is recovered by letting $[W]^T = [B]^T$ in (34). Interestingly, note that other weighting functions may lead to solutions that do not comply with the second law of thermodynamics. Specifically, if another choice of weighting function is used in equation (34), it no longer follows from the dissipation inequality, equation (29), that $\{\delta d^p\}^T \int_V [B]^T \left\{ \frac{\partial \psi}{\partial \epsilon^p} \right\} dV \leq 0$. Hence, it is possible the model will predict the free energy generated exceeds the work done on the element, that is, $\delta\psi > \delta W$.

4 Conclusion

Recent advances in the development of constitutive models of complex and heterogeneous materials have been based on Cosserat or micropolar theory

as well as other "enriched" continua. These models have generated new perspectives and concepts which are only now beginning to be systematically examined. In particular, a key challenge confronting modellers of these new breed of constitutive models is the need to check, retroactively, that these models are indeed consistent with the laws of thermodynamics. However, in the thermomechanical approach, compliance with thermodynamics is guaranteed at the outset, since constitutive relations are derived directly from the laws of thermodynamics.

We have shown how the thermomechanical approach can also be applied to the formulation of finite element models of micropolar continua undergoing both elastic and plastic deformations. This technique then offers the added advantage that the implementation phase of the model is linked directly to the underlying physics. Tordesillas et al. [9] and Tordesillas and Walsh [11] discuss examples of this approach applied to specific material models. An interesting finding borne out by this analysis is that while the traditional Galerkin method admits a range of weighting functions, the second law of thermodynamics provides an additional constraint that narrows the choice of admissible weighting functions. In particular, we have shown that the second law of thermodynamics is satisfied if the weighting function is given by the strain-displacement matrix: other weighting functions may not guarantee compliance with this law.

Finally, while we have only considered micropolar materials in this paper, we anticipate that more complex microdeformation (Eringen [3]) can be accounted for using the same principles.

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