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SIMULATION OF DISCONTINUITY MOVEMENT BY BOUNDARY ELEMENTS

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Summary A numerical scheme which describes the movement of a discontinuity in a continuum is presented. The local behavior governing the propagation of the discontinuity as well as the behavior of the bulk material is considered. The same discretization is used for the description of the interface propagation and the bulk behavior by employing a moving finite element scheme ([1]) and the boundary element method. Results obtained using a three dimensional implementation of the scheme described above for a phase transformation problem are presented.

INTRODUCTION

For problems involving the movement of a discontinuity in a continuum, the explicit knowledge of its position is often of vital importance for the numerical simulation of the material response. The movement of this discontinuity can usually be expressed in terms of the state in its direct vicinity. However, the local state at the discontinuity may be heavily influenced by the behavior of the bulk material. Thus, for an accurate description of the material response, both aspects may have to be taken into account.

MATERIAL BEHAVIOR

The procedure leading to the identification of the driving force for the movement of the discontinuity is described by numerous authors (see e.g. [3]). In the following, a jump at the discontinuity is denoted by $[\bullet]$. The term

$$T\dot{s}_\Lambda = \rho\dot{l}\ \boldsymbol{n}\cdot[\boldsymbol{\mu}]\cdot\boldsymbol{n}\ \geq 0 \tag{1}$$

is identified as the term describing the local dissipation $\dot{s}_\Lambda$ due to the movement of the discontinuity. $\boldsymbol{n}$ denotes the normal vector to the discontinuity, ρ the mass-density, and $\dot{l}$ the normal velocity of the propagating interface, all terms in the referential description. T denotes the absolute temperature. Furthermore,

$$\boldsymbol{\mu} := \varphi\,\mathbf{1} - \frac{1}{\rho}\,\mathbf{C}\cdot\mathbf{S} \tag{2}$$

has been introduced. φ denotes the specific free Helmholtz energy, $\mathbf{1}$ the second-order unit-tensor in the referential description, $\mathbf{C}$ the right Cauchy-Green tensor, and $\mathbf{S}$ the second Piola-Kirchhoff stress. It is noteworthy that the transpose of $\boldsymbol{\mu}$ is often denoted "Eshelby-Tensor". As this tensor is always used in conjunction with a projection in direction of the normal $\boldsymbol{n}$ (i.e. $\boldsymbol{n}\cdot\boldsymbol{\mu}\cdot\boldsymbol{n}$), the asymmetric part of $\boldsymbol{\mu}$ does not influence this problem and the difference of the descriptions is not of importance. Heidug and Lehner have shown in [3] that the condition $\boldsymbol{n}\cdot[\boldsymbol{\mu}]\cdot\boldsymbol{n} = 0$ is a necessary condition for unconstrained thermodynamic equilibrium, i.e. for the absence of movement of the discontinuity. Thus, the projection of the tensor $\boldsymbol{\mu}$ can be interpreteded as the thermodynamic force for the local movement of the discontinuity and may be used in a concept which describes locally the movement of the discontinuity. A linear relation between the thermodynamic driving force and the movement of the interface $\dot{l}$ is used here (cf. [5]), i.e.

$$\dot{l} - c\,\boldsymbol{n}\cdot[\boldsymbol{\mu}]\cdot\boldsymbol{n} = 0 \tag{3}$$

with the constant parameter $c > 0$. This ensures the validity of equation (1). For the bulk, a linear elastic isotropic behavior is assumed.

NUMERICAL REALIZATION

For simplicity, the behavior of the bulk material and the interface movement are treated independently for the current time step. For the time t, the BEM-solution delivers the terms to calculate the vector F_I, which is derived later. The interface-evolution step is performed advancing the solution by the time step Δt, leading to a new position of the interface. Then again, the BEM-procedure is used and so on. Furthermore, it is assumed that small strain procedures are sufficient.

Description of the Interface Movement

The position vector of a point on the interface is denoted by $\boldsymbol{r}$. In the current implementation, only the movement of the interface normal to itself is considered, hence

$$\dot{\boldsymbol{r}} = \boldsymbol{n}\,\dot{l}. \tag{4}$$

An additional term $\boldsymbol{n}^*\,l^*$ with $\boldsymbol{n}^*\cdot\boldsymbol{n} = 0$ may be added later to avoid a degeneration of the mesh. The weak form of equation (3) can be derived by introducing a trial function $\boldsymbol{r}^*$, reading

$$\int_\Lambda \boldsymbol{r}^*\cdot\dot{\boldsymbol{r}}\,\mathrm{d}A = \int_\Lambda c\,(\boldsymbol{r}^*\cdot\boldsymbol{n})\,(\boldsymbol{n}\cdot[\boldsymbol{\mu}]\cdot\boldsymbol{n})\,\mathrm{d}A \tag{5}$$

where $\int_\Lambda \bullet \, \mathrm{d}A$ denotes the integration over the interface. Using the approximations

$$\boldsymbol{r}(\boldsymbol{x},t) = \sum_I \mathbf{N}_I(\boldsymbol{x})\, r_I(t) \quad \text{and} \quad \boldsymbol{r}^*(\boldsymbol{x},t) = \sum_I \mathbf{N}_I(\boldsymbol{x})\, r_I^*(t) \tag{6}$$

with the shape functions $\mathbf{N}_I(\boldsymbol{x})$ provided by the boundary element method ($\boldsymbol{x}$ may be interpreted as the initial position of the point considered, i.e. $\boldsymbol{x} = \boldsymbol{r}(\boldsymbol{x},0)$) leads to

$$\sum_I \sum_J r_I^* \int_\Lambda \mathbf{N}_I \cdot \mathbf{N}_J \, \mathrm{d}A \, \dot{r}_J = \sum_I r_I^* \int_\Lambda c \, (\mathbf{N}_I \cdot \boldsymbol{n}) \, (\boldsymbol{n} \cdot [\boldsymbol{\mu}] \cdot \boldsymbol{n}) \, \mathrm{d}A. \tag{7}$$

As equation (7) holds for arbitrary $\boldsymbol{r}^*$, it can be expressed as

$$\sum_J D_{IJ} \, \dot{r}_J = F_I \tag{8}$$

using the abbreviations

$$D_{IJ} = \int_\Lambda \mathbf{N}_I \cdot \mathbf{N}_J \, \mathrm{d}A \quad \text{and} \quad F_I = \int_\Lambda c \, (\mathbf{N}_I \cdot \boldsymbol{n}) \, (\boldsymbol{n} \cdot [\boldsymbol{\mu}] \cdot \boldsymbol{n}) \, \mathrm{d}A. \tag{9}$$

Explicit and implicit integration schemes (cf. [6]) are used to integrate equation (8).

Description of the Bulk Material

The boundary element description used to approximate the behavior of the bulk material is based on the code described in [7]. The code is extended to handle a spatially varying additional deformation following the initial strain approach (cf. [2]). For each domain of the material, a discretization of its boundary is used. Consequently, usual boundary element matrices can be formulated and combined to solve the overall mechanical problem.

EXAMPLES

The influence of the choice of the time step Δt on stability and computational cost is studied by some simple examples for the explicit and implicit integration schemes.

As a more illustrative example, the propagation of phase transformation front in a NiTi single crystal is considered. The crystallographic theory of martensite ([4]) is followed to determine the active martensite variants in the transformation layer. For a Ti-rich alloy, the influence of a Ti-inclusion on the overall transformation behavior during a differential scanning calometry test is investigated.

References

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