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A time-integration scheme for thermomechanical evolutions of shape-memory alloys

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Abstract

This Note presents a time-integration strategy for computing the evolution of structures embedding shape-memory alloys in a thermomechanical setting. A variational formulation is associated with the scheme proposed, which allows one to study the existence and unicity of solutions depending on the material model considered. A numerical example is presented to illustrate the method and discuss the influence of the thermomechanical coupling. ***To cite this article: M. Peigney, C. R. Mecanique 334 (2006).***

Résumé

Un algorithme d'intégration en temps pour l'évolution thermomécanique des alliages à mémoire de forme. Cette Note présente un algorithme d'intégration en temps pour l'évolution thermomécanique des structures formées d'alliages à mémoire de forme. On donne une formulation variationnelle du problème discrétisé en temps, ce qui permet d'étudier l'existence et l'unicité de solutions en fonction de la loi de comportement utilisée. Un exemple numérique est présenté afin d'illustrer la méthode et d'étudier l'influence du couplage thermomécanique. ***Pour citer cet article : M. Peigney, C. R. Mecanique 334 (2006).***

Keywords: Solids and structures; Shape-memory alloys; Phase transformation; Thermomechanical coupling; Numerical algorithms

Mots-clés : Solides et structures ; Alliages à mémoire de forme ; Transformation de phase ; Couplage thermomécanique ; Algorithmes numériques

1. Introduction

The peculiar properties of Shape Memory Alloys (SMAs) are connected to the solid–solid phase transformation between austenite and martensite. Those materials have been extensively studied in the context of quasi-static evolutions, supposing that the system is in thermal equilibrium at each time. The phase transformation in SMAs is known to produce heat (recoverable latent heat and irreversible frictional contributions), and the validity of the thermal equilibrium assumption is in fact dependent on the rate of loading and on the thermal exchange conditions between the system and its environment. To better predict the response of SMA systems, it is therefore necessary to take the thermomechanical coupling into account, considering the temperature field as an unknown to be solved for. The time-discretization of

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the system obtained is not obvious, and difficulties of convergence have been observed in numerical simulations (see, e.g., [1]). The purpose of this Note is to propose a time-discretization scheme for which existence of solutions to the incremental problem is ensured for a large class of SMA material models.

2. Local equations

The analysis is conducted in the context of small perturbations. The displacement, stress and temperature are denoted by $\boldsymbol{v}$, $\boldsymbol{\sigma}$ and θ respectively. Some internal variables $\boldsymbol{\beta}$ are introduced to account for the phase transformation. In most models found in the literature, $\boldsymbol{\beta}$ represents the volume fractions of the different variants of martensite. Those internal variables are required to belong to a closed and convex set $\mathcal{T}$ representing constraints on $\boldsymbol{\beta}$. For instance, if $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_n)$ where β_i is the volume fraction of the variant i of martensite, then $\mathcal{T}$ is given by $\{\boldsymbol{\beta} \mid \beta_i \geqslant 0;\ \sum_{i=1}^n \beta_i \leqslant 1\}$. As pointed out by Frémond [2], the presence of such constraints implies that the mechanical quantities are not necessarily differentiable with respect to time. Following Frémond [2], we will suppose that left-derivatives exist for the quantities considered. All the time-derivatives in the following are left-derivatives.

The system occupies a volume Ω, in which a body force $\boldsymbol{f}^d$ is imposed. Tractions $\boldsymbol{T}^d$ are given on a part Γ^T of the boundary $\partial\Omega$, while displacements $\boldsymbol{v}^d$ are imposed on $\Gamma^v = \partial\Omega - \Gamma^T$. The temperature is set equal to θ^d on a portion Γ_θ of $\partial\Omega$, and the heat flux q_N^d is imposed on a portion Γ_q such that $\Gamma_q \cap \Gamma_\theta = \emptyset$. On the remaining part $\Gamma_r = \partial\Omega - \Gamma_\theta - \Gamma_q$ of the boundary, the heat flux is given by $K'(\theta - \theta_R)$ where K' is a (positive) heat transfer coefficient between the system and its environment. In the volume Ω, the heat flux $\boldsymbol{q}$ is supposed to satisfy the Fourier's law $\boldsymbol{q} = -K\nabla\theta$ where K is the thermal conductivity. The functions $\boldsymbol{f}^d$, $\boldsymbol{T}^d$, $\boldsymbol{v}^d$, θ^d, q_N^d describing the thermomechanical loading depend on the position $\boldsymbol{x}$ and on the time t.

The principle of virtual power and the two principles of thermodynamics yield a general form for the equations governing the system. This analysis must be carried out in the framework of non-smooth mechanics (see [2]) to account for the constraints on $\boldsymbol{\beta}$. The resulting equations are

$$\boldsymbol{\sigma} = \frac{\partial w}{\partial \boldsymbol{\varepsilon}}, \qquad \boldsymbol{B} = -\frac{\partial w}{\partial \boldsymbol{\beta}}, \qquad s = -\frac{\partial w}{\partial \theta} \tag{1.1}$$

$$\boldsymbol{\varepsilon} = (\nabla\boldsymbol{v} + {}^t\nabla\boldsymbol{v})/2 \tag{1.2}$$

$$\boldsymbol{B} = \boldsymbol{B}^r + \boldsymbol{B}^d \tag{1.3}$$

$$-K\frac{\partial\theta}{\partial\boldsymbol{n}} = q_N^d \quad \text{on } \Gamma_q, \qquad -K\frac{\partial\theta}{\partial\boldsymbol{n}} = K'(\theta - \theta_R) \quad \text{on } \Gamma_r \tag{1.4}$$

$$\boldsymbol{v} \in \mathcal{K}_v, \qquad \boldsymbol{\sigma} \in \mathcal{K}_\sigma, \qquad \theta \in \mathcal{K}_\theta \tag{1.5}$$

$$\boldsymbol{B}^r \in \partial I_{\mathcal{T}}(\boldsymbol{\beta}), \qquad \boldsymbol{B}^d \in \partial\Phi(\dot{\boldsymbol{\beta}}) \tag{1.6}$$

$$\boldsymbol{B}^d.\dot{\boldsymbol{\beta}} - \theta\dot{s} + K\Delta\theta = 0 \tag{1.7}$$

where the sets $\mathcal{K}_v$,$\mathcal{K}_\sigma$,$\mathcal{K}_\theta$ are defined by

$$\begin{aligned} &\mathcal{K}_v = \{\boldsymbol{v} \mid \boldsymbol{v} = \boldsymbol{v}^d \text{ on } \Gamma^v\}, \qquad \mathcal{K}_\sigma = \{\boldsymbol{\sigma} \mid \operatorname{div}\boldsymbol{\sigma} + \boldsymbol{f}^d = 0 \text{ in } \Omega;\ \boldsymbol{\sigma}.\boldsymbol{n} = \boldsymbol{T}^d \text{ on } \Gamma^T\}, \\ &\mathcal{K}_\theta = \{\theta \mid \theta = \theta^d \text{ on } \Gamma_\theta\} \end{aligned} \tag{2}$$

In (1), $I_{\mathcal{T}}$ is the indicator function of the set $\mathcal{T}$ (i.e., null in $\mathcal{T}$ and infinite outside $\mathcal{T}$), w is the free energy and the dissipation potential Φ is a convex positive function such that $\Phi(0) = 0$. The notation ∂ denotes the subdifferential (see [3]). Several expressions have been proposed for w and Φ. For latter reference, we consider as an example the model of Anand and Gurtin [4], defined by

$$\begin{aligned} &w(\boldsymbol{\varepsilon}, \boldsymbol{\beta}, \theta) = \frac{1}{2}\left(\boldsymbol{\varepsilon} - \sum_{i=1}^n \beta_i \boldsymbol{\varepsilon}_i^{\mathrm{tr}}\right) : \boldsymbol{L} : \left(\boldsymbol{\varepsilon} - \sum_{i=1}^n \beta_i \boldsymbol{\varepsilon}_i^{\mathrm{tr}}\right) + \frac{\lambda_T}{\theta_T}(\theta - \theta_T)\left(\sum_{i=1}^n \beta_i\right) + c(\theta - \theta_R) - c\theta\log(\theta/\theta_R) \\ &\Phi(\dot{\boldsymbol{\beta}}) = G\sum_{i=1}^n |\dot{\beta}_i| \end{aligned} \tag{3}$$

This model considers n variants of martensite, each variant being characterized by its volume fraction β_i and its transformation strain $\boldsymbol{\varepsilon}_i^{\mathrm{tr}}$. The tensor $\boldsymbol{L}$ is the symmetric positive definite elasticity tensor, λ_T is the latent heat at temperature θ_T, c is the specific heat and θ_R is a reference temperature. The positive parameter G determines the mechanical dissipation.

3. Simplification of the heat equation

The heat equation (1.7) can be rewritten as

$$K\Delta\theta + \theta\frac{\partial^2 w}{\partial\theta\partial\boldsymbol{\varepsilon}}\dot{\boldsymbol{\varepsilon}} + \theta\frac{\partial^2 w}{\partial\theta^2}\dot{\theta} + \left(\theta\frac{\partial^2 w}{\partial\theta\partial\beta} + \boldsymbol{B}^d\right).\dot{\boldsymbol{\beta}} = 0 \tag{4}$$

The last term in this equation can be interpreted as a heat source created by the phase transformation. This source breaks up in two parts: the heat $S_1 = \boldsymbol{B}^d.\dot{\boldsymbol{\beta}}$ associated with the dissipative behaviour, and the recoverable latent heat $S_2 = \theta\dot{\boldsymbol{\beta}}.\frac{\partial^2 w}{\partial\theta\partial\beta}$. Experimental evidence (see, e.g., [5]) shows that S_1 is small compared to S_2. Let us give some indicative figures using the model of Anand and Gurtin [4]: in this model, S_1 is equal to $\sum_i G|\dot{\beta}_i|$ and S_2 is equal to $\lambda_T(\theta/\theta_T)\sum_i\dot{\beta}_i$. Typical values of $(G, \lambda_T, \theta, \theta_T)$ given in [4] are $G = 4.7$ MPa, $\lambda_T = 110$ MPa, $\theta = 300$ K, $\theta_T = 271$ K. This leads to $|S_1/S_2| < 3.9\%$.

In such a framework, it is reasonable to drop the term $S_1 = \boldsymbol{B}^d.\dot{\boldsymbol{\beta}}$ in the heat equation, which therefore simplifies as

$$K\Delta\theta - \theta\dot{s} = 0 \tag{5}$$

4. Introduction of a finite time-step problem

We now address the time discretization of the system formed by Eqs. (1.1)–(1.6) along with (5). Supposing that the fields $\boldsymbol{v}^0$, $\boldsymbol{\beta}^0$, θ^0 at time t^0 are known, the problem is to determine the fields $\boldsymbol{v}$, $\boldsymbol{\beta}$, θ at time $t^0 + \delta t$ with $\delta t > 0$. To this purpose, we propose to estimate $\boldsymbol{v}$, $\boldsymbol{\beta}$, θ by solving the following problem:

$$(\boldsymbol{v}, \boldsymbol{\beta}, \theta) \text{ verify (1.1)–(1.5) at time } t^0 + \delta t \tag{6.1}$$

$$\boldsymbol{B}^r \in \partial I_{\mathcal{T}}(\boldsymbol{\beta}), \qquad \boldsymbol{B}^d \in \partial\Phi\big((\boldsymbol{\beta} - \boldsymbol{\beta}^0)/\delta t\big) \tag{6.2}$$

$$K\delta t\left[\Delta\theta + \frac{\nabla\theta^0}{\theta^0}.\nabla(\theta^0 - \theta)\right] - \theta^0(s - s^0) = 0 \tag{6.3}$$

where $s^0 = s(\boldsymbol{\varepsilon}^0, \boldsymbol{\beta}^0, \theta^0)$.

It should be verified that (6.3) is a time-discretization of (5) in the sense that (6.3) coincides with (5) in the limit $\delta t \to 0$. To do so, let us substitute in (6.3) the following development:

$$\theta = \theta^0 + \dot{\theta}\delta t + \mathrm{o}(\delta t), \qquad s = s^0 + \dot{s}\delta t + \mathrm{o}(\delta t) \tag{7}$$

We find

$$K\delta t\left(\Delta\theta^0 + \delta t\Delta\dot{\theta} - \frac{\nabla\theta^0}{\theta^0}\nabla\dot{\theta}\delta t\right) - \theta^0\dot{s}\delta t + \mathrm{o}(\delta t) = 0 \tag{8}$$

Dividing by δt and taking the limit $\delta t \to 0$ shows that

$$K\Delta\theta^0 - \theta^0\dot{s} = 0 \tag{9}$$

This proves that (6.3) is a time-discretization of the heat equation (5), although not as intuitive as the standard implicit time-discretization of (5), given by:

$$K\delta t\Delta\theta - \theta^0(s - s^0) = 0 \tag{10}$$

Motivation of the scheme (6) is that a variational formulation can be given.

5. Variational formulation of the finite time-increment problem

We denote by $\mathcal{K}_\beta$ the set of fields $\boldsymbol{\beta}$ such that $\boldsymbol{\beta}(\boldsymbol{x}) \in \mathcal{T}$ for all $\boldsymbol{x}$ in Ω. We introduce a functional $\mathcal{F}$ defined on the convex set $\mathcal{K}_v \times \mathcal{K}_\beta \times \mathcal{K}_\theta$ by

$$\begin{aligned}\mathcal{F}(\boldsymbol{v},\boldsymbol{\beta},\theta) = {} & \int_\Omega w\big(\boldsymbol{\varepsilon}(\boldsymbol{v}),\boldsymbol{\beta},\theta\big)\,\mathrm{d}\omega - \int_\Omega \boldsymbol{f}^d.\boldsymbol{v}\,\mathrm{d}\omega - \int_{\Gamma^T} \boldsymbol{T}^d.\boldsymbol{v}\,\mathrm{d}a + \delta t \int_\Omega \Phi\big((\boldsymbol{\beta}-\boldsymbol{\beta}^0)/\delta t\big)\,\mathrm{d}\omega \\ & + \int_\Omega \theta s^0\,\mathrm{d}\omega + \delta t \int_\Omega K\left(-\frac{1}{2}\frac{1}{\theta^0}\|\nabla\theta\|^2 + \left(\frac{\|\nabla\theta^0\|}{\theta^0}\right)^2\theta\right)\mathrm{d}\omega \\ & - \delta t \int_{\Gamma_q} \frac{q_N^d}{\theta^0}\theta\,\mathrm{d}a - K'\frac{\delta t}{2}\int_{\Gamma_r}\frac{(\theta-\theta_R)^2}{\theta^0}\,\mathrm{d}a \end{aligned} \tag{11}$$

The solutions of (6) are the solutions of the following problem:

Find $(\boldsymbol{v},\boldsymbol{\beta},\theta) \in \mathcal{K}_v \times \mathcal{K}_\beta \times \mathcal{K}_\theta$ such that for all $(\boldsymbol{v}^*,\boldsymbol{\beta}^*,\theta^*) \in \mathcal{K}_v \times \mathcal{K}_\beta \times \mathcal{K}_\theta$:

$$0 \leqslant \frac{\partial\mathcal{F}}{\partial\boldsymbol{v}}(\boldsymbol{v}^*-\boldsymbol{v}) + \frac{\partial\mathcal{F}}{\partial\boldsymbol{\beta}}(\boldsymbol{\beta}^*-\boldsymbol{\beta}) + \frac{\partial\mathcal{F}}{\partial\theta}(\theta^*-\theta) \tag{12}$$

Let us briefly justify this result: writing down the stationary conditions in (12) with respect to $\boldsymbol{v}^*$ give the equations $\boldsymbol{\sigma} = \partial w/\partial\boldsymbol{\varepsilon}$ and $\boldsymbol{\sigma} \in \mathcal{K}_\sigma$. The stationary conditions with respect to θ^* are found to give the relations (1.4) and (6.3) by use of the following identity:

$$-\int_\Omega \frac{\nabla\theta}{\theta^0}.\nabla(\delta\theta)\,\mathrm{d}\omega = \int_\Omega \mathrm{div}\left(\frac{\nabla\theta}{\theta^0}\right)\delta\theta\,\mathrm{d}\omega - \int_{\partial\Omega}\delta\theta\frac{\nabla\theta}{\theta^0}.\boldsymbol{n}\,\mathrm{d}a \tag{13}$$

Now taking $\boldsymbol{v}^* = \boldsymbol{v}$ and $\theta^* = \theta$ in (12), we obtain

$$-\boldsymbol{B}.(\boldsymbol{\beta}^*-\boldsymbol{\beta}) + \delta t\Phi\big((\boldsymbol{\beta}^*-\boldsymbol{\beta}^0)/\delta t\big) - \delta t\Phi\big((\boldsymbol{\beta}-\boldsymbol{\beta}^0)/\delta t\big) \geqslant 0 \quad \text{for all } \boldsymbol{\beta}^* \in \mathcal{T} \tag{14}$$

Consider the convex functions ϕ and ψ defined respectively by $\phi(\boldsymbol{\beta}') = \delta t\Phi((\boldsymbol{\beta}'-\boldsymbol{\beta}^0)/\delta t)$ and $\psi(\boldsymbol{\beta}') = \phi(\boldsymbol{\beta}') + I_\mathcal{T}(\boldsymbol{\beta}')$ for all $\boldsymbol{\beta}'$ (not necessarily in $\mathcal{T}$). We have $-\boldsymbol{B}.\delta\boldsymbol{\beta} + \psi(\boldsymbol{\beta}+\delta\boldsymbol{\beta}) - \psi(\boldsymbol{\beta}) \geqslant 0$ for all $\delta\boldsymbol{\beta}$, which means that $\boldsymbol{B}$ belongs to the subdifferential $\partial\psi(\boldsymbol{\beta})$. Note that ϕ is a proper convex lower semi-continuous function. The function $I_\mathcal{T}$ is also proper, lower semi-continuous, and convex because $\mathcal{T}$ is a non-empty, closed, convex set. It follows from a classical result of convex analysis (see [3]) that $\partial\psi = \partial(\phi + I_\mathcal{T}) = \partial\phi + \partial I_\mathcal{T}$. Therefore, any $\boldsymbol{B}$ satisfying (14) verifies (6.2).

The variational formulation (12) allows one to study the existence and unicity of solutions for the time-integrated problem (6). Suppose in particular that w is convex with respect to $(\boldsymbol{v},\boldsymbol{\beta})$ and concave with respect to θ. Then the functional $\mathcal{F}$ is convex with respect to the fields $(\boldsymbol{v},\boldsymbol{\beta})$ and concave with respect to the field θ, so that a saddle point exists (provided adequate functional spaces are chosen for $\mathcal{K}_v$, $\mathcal{K}_\beta$ and $\mathcal{K}_\theta$). Such a saddle point $(\boldsymbol{v},\boldsymbol{\beta},\theta)$ verifies (12) and therefore is solution of (6). If there is strict convexity and concavity, this saddle point is unique.

In the model of Anand and Gurtin [4], the free energy w is given by (3) and therefore is convex in $(\boldsymbol{\varepsilon},\boldsymbol{\beta})$ and concave in θ. Consequently, the problem (6) has a solution. Notice that $\mathcal{F}$ is not strictly convex in $(\boldsymbol{\varepsilon},\boldsymbol{\beta})$, so unicity of the solution to (6) is not ensured.

As another example, let us consider the model of Auricchio and Petrini [6], in which the internal variable $\boldsymbol{\beta}$ is a symmetric tensor corresponding to the transformation strain. Using the expressions given in [6], it can be verified that the free energy in this model is strictly convex with respect to $(\boldsymbol{\varepsilon},\boldsymbol{\beta})$ and strictly concave with respect to θ, as long as θ remains in the superelastic regime (defined by $\theta > M_f$ for a characteristic temperature M_f considered in [6]). In this setting, the existence and unicity of a solution to the finite-step incremental problem (6) is guaranteed.

Remark 1. When the temperature field θ is assumed to be known, the functional $\mathcal{F}$ to consider reduces to the first line of (11). This essentially corresponds to the incremental variational formulation introduced by Miehe et al. [7] for studying isothermal evolutions of inelastic materials.

Remark 2. So far Φ has been considered as independent on θ. When Φ depends both on $\dot{\boldsymbol{\beta}}$ and θ, the term $\partial\Phi$ in (1.6) and (6.2) is replaced by the partial derivative $\partial_{\dot{\boldsymbol{\beta}}}\Phi$. If $\Phi(\dot{\boldsymbol{\beta}},\theta)$ can be written as $f(\theta\dot{\boldsymbol{\beta}})$ for some differentiable function f, then the solutions of (12) are found to be solutions of (6.1), (6.2) together with the following equation:

$$K\delta t\left[\Delta\theta+\frac{\nabla\theta^0}{\theta^0}.\nabla(\theta^0-\theta)\right]-\theta^0(s-s^0)+\frac{\theta^0}{\theta}(\boldsymbol{\beta}-\boldsymbol{\beta}^0).\partial_{\dot{\boldsymbol{\beta}}}\Phi\left(\theta,\frac{\boldsymbol{\beta}-\boldsymbol{\beta}^0}{\delta t}\right)=0 \tag{15}$$

This equation is a time-discretization of the fully coupled heat equation (1.7): in this case, the variational problem (12) allows one to tackle the fully coupled thermomechanical evolution.

6. Numerical example

The approach presented is used in conjunction with the model of Anand and Gurtin [4] to simulate the propagation of a martensitic zone in a circular cylinder under traction. As the loading increases with time, transformation into martensite takes place. For estimating the solution at $t^0+\delta t$ starting from the solution at t^0, a simple numerical strategy consists in solving the incremental mechanical and thermal problems successively until convergence. When the heat equation is discretized in a standard implicit form (10), neither the convergence of this iterative process nor the existence of a solution is ensured. When the heat equation is instead discretized in the form (6.3) as proposed, a solution to the incremental problem does exist and the iterative process can be interpreted as a relaxation algorithm for finding a saddle point of $\mathcal{F}$. The number of iterations necessary to reach convergence with each one of these discretizations is shown on Table 1. This results show that the method proposed allows for better computational costs.

The solid-line curve on Fig. 1 shows the total volume fraction of martensitic as a function of the displacement imposed u^d. The dashed-line curve on Fig. 1 corresponds to the case where thermal effects are neglected: that isothermal computation overestimates the total volume fraction of martensite by about 20%. This illustrates the importance of taking the thermomechanical coupling into account.

Table 1
Number of iterations for solving the incremental problem

δt (s)	10^{-4}	2×10^{-4}	10^{-3}	2×10^{-3}
Standard discretization	9	11	17	16
Modified discretization	7	8	8	10

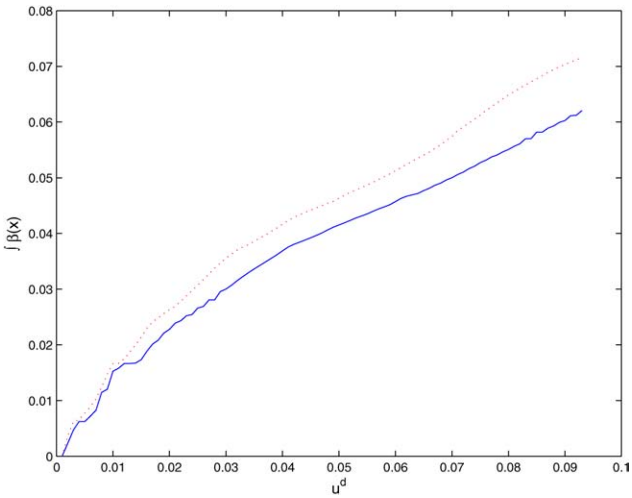

Fig. 1. Evolution of the total volume fraction of martensite.

7. Conclusion

A robust time-integration scheme has been introduced for computing thermomechanical evolutions of SMAs. A central point in the analysis is the fact that, in SMAs, the irreversible heat contribution is small compared to the latent heat contribution. This enables one to write down a finite time-step evolution problem which can be formulated as a saddle point problem. Such a variational formulation is in itself an improvement on the standard approach, as existence of solutions to the finite time-step problem can be proved and better numerical convergence is observed. This variational formulation is a first step towards studying the convergence of the time-discretized approximations towards solutions of the time-continuous evolution problem.

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