XI International Conference on Computational Plasticity. Fundamentals and Applications
COMPLAS XI
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THERMOMECHANICAL SIMULATION OF SHAPE MEMORY ALLOYS STRUCTURES: VARIATIONAL METHODS AND ASSOCIATED NUMERICAL TOOLS

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Key words: Computational Plasticity, Shape memory alloys, Thermomechanical coupling, Linear complementarity problem

Abstract. Shape Memory Alloys (SMA) offer new perspectives in various fields such as aeronautics, robotics, biomedicals, or civil engineering. Efficient design of such innovative systems requires both adequate material models and numerical methods for simulating the response of SMA structures. Whereas much effort has been devoted to developing constitutive laws for describing the behaviour of SMAs, the structural problem (i.e. the simulation of a three-dimensional SMA structure) has received far less attention, in spite of substantial difficulties notably due to the strong thermomechanical coupling and the presence of physical constraints on the internal variables. The time-discretization of the evolution problem obtained is not obvious, and special care must be taken to avoid convergence difficulties and ensure robustness of the numerical schemes. Computation time and ease of implementation (for instance in an existing finite element code) also are major issues that need to be addressed. In this communication are presented some recent results in that direction. A central result is a recent time-discretization scheme for the thermomechanical problem. A variational formulation is attached to the corresponding incremental problem, allowing one to prove the existence of solutions for a large class of usual SMA models. The variational nature of the problem at hand also calls for an easy implementation in an existing finite element code, building on well-established descend algorithms. Using that approach, the solution of the thermomechanical incremental problem is typically obtained by solving a sequence of linear thermal problems and purely mechanical (i.e. at prescribed temperature) nonlinear problems. That approach is fairly general and applies for a wide range of SMA models. The numerical scheme for solving the purely mechanical problem, however, strongly depends on the particular model that is used. In a micromechanical modelling of SMAs, the phase transformation is described locally by an internal vectorial variable which is physically constrained to satisfy a set of inequalities at each point. We show that the corresponding incremental problem can

be recast as a linear complementarity problem, for which efficient algorithms (such as interior-point methods) are available. That reformulation essentially consists in a change of variables. In terms of variational formulation, that approach amounts to replace a convex but non-quadratic minimization problem with an equivalent quadratic minimization problem.

1 COUPLED THERMOMECHANICAL EVOLUTIONS

We consider the evolution problem of an arbitrary SMA structure, in quasi-statics and under the assumption of small strains. The structure occupies a domain Ω and is submitted to body forces $\boldsymbol{f}^d$ and tractions $\boldsymbol{T}^d$, the latter being applied on a portion Γ^T of the boundary. Prescribed displacements $\boldsymbol{u}^d$ are imposed on $\Gamma^U = \partial\Omega - \Gamma^T$. The temperature θ is set equal to θ^d on a portion Γ_θ of $\partial\Omega$, and the heat flux q^d is imposed on a portion Γ_q such that $\Gamma_q \cap \Gamma_\theta = \emptyset$. On the remaining part $\Gamma_r = \partial\Omega - \Gamma_q - \Gamma_\theta$ 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. The functions $\boldsymbol{f}^d$, $\boldsymbol{T}^d$, $\boldsymbol{u}^d$, θ^d, q^d describing the thermomechanical loading depend on the position $\boldsymbol{x}$ and on the time t. In the domain Ω, the heat flux $\boldsymbol{q}$ is supposed to satisfy the Fourier's law with a thermal conductivity K. The displacement, stress and temperature are denoted by $\boldsymbol{u}$, $\boldsymbol{\sigma}$ and θ respectively.

In a mesoscopic modelling of SMAs, the local state of the material is described by the variables ($\boldsymbol{\varepsilon}$, $\boldsymbol{\xi}$, θ) where $\boldsymbol{\varepsilon}$ is a strain and $\boldsymbol{\xi}$ is a (possibly vectorial) internal variable tracking the phase transformation. That variable $\boldsymbol{\xi}$ must generally satisfy a condition of the form $\boldsymbol{\xi} \in \mathcal{T}$ where $\mathcal{T}$ is a given bounded set (see Section 3 for an explicit example). Denoting the free energy of the material by w and the dissipation potential by ϕ, the evolution of the system is governed by the following system (see [2] and references therein for more details) :

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

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

$$-K\nabla\theta.\boldsymbol{n} = q^d \text{ on } \Gamma_q, \ -K\nabla\theta.\boldsymbol{n} = K'(\theta - \theta_R) \text{ on } \Gamma_r \tag{1.3}$$

$$\boldsymbol{u} \in \mathcal{K}_u \ , \boldsymbol{\sigma} \in \mathcal{K}_\sigma \ , \ \boldsymbol{\xi} \in \mathcal{K}_\xi \ , \ \theta \in \mathcal{K}_\theta \tag{1.4}$$

$$\boldsymbol{B} = \boldsymbol{B}^r + \boldsymbol{B}^d \tag{1.5}$$

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

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

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

$$\begin{array}{rcl} \mathcal{K}_u & = & \{\boldsymbol{u} | \boldsymbol{u} = \boldsymbol{u}^d \text{ on } \Gamma^u\} \\ \mathcal{K}_\sigma & = & \{\boldsymbol{\sigma} | \operatorname{div} \boldsymbol{\sigma} + \boldsymbol{f}^d = 0 \text{ in } \Omega; \boldsymbol{\sigma}.\boldsymbol{n} = \boldsymbol{T}^d \text{ on } \Gamma^T\} \\ \mathcal{K}_\xi & = & \{\boldsymbol{\xi} | \boldsymbol{\xi} \in \mathcal{T} \text{ in } \Omega\} \\ \mathcal{K}_\theta & = & \{\theta | \theta = \theta^d \text{ on } \Gamma_\theta\} \end{array} \tag{2}$$

In (1), $I_\mathcal{T}$ is the indicator function of the set $\mathcal{T}$ (equal to 0 in and infinite outside) et ∂ denotes the subdifferential [1]. In the heat equation (1.7), the thermomechanical coupling is embedded both in the entropy-related term $\theta \dot{s}$ (which contains the latent heat effect) and in the dissipative term $\boldsymbol{B}^d.\dot{\boldsymbol{\xi}}$.

2 TIME-DISCRETIZATION OF THE EVOLUTION PROBLEM

2.1 Incremental problem

To solve a system such (1), one generally resorts to a space- and time-discretization strategy. The space discretization is generally supplied by a finite element method. The time discretization consists in introducing a finite time-step problem for estimating the solution $(\boldsymbol{u}, \boldsymbol{\sigma}, \theta)$ at a given time $t^0 + \delta t$, supposing that $(\boldsymbol{u}^0, \boldsymbol{\sigma}^0, \theta^0)$ at time t^0 are known. For the system considered, a common finite time-step problem is supplied by the backwards Euler scheme, which can be formulated as follows:

$$(\boldsymbol{u}, \boldsymbol{\xi}, \theta) \text{ verifies (1.1)-(1.4) at } t^0 + \delta t \tag{3.1}$$

$$\boldsymbol{B} = \boldsymbol{B}^r + \boldsymbol{B}^d \tag{3.2}$$

$$\boldsymbol{B}^r \in \partial I_\mathcal{T}(\boldsymbol{\xi}) \ , \ \boldsymbol{B}^d \in \partial \phi\big((\boldsymbol{\xi} - \boldsymbol{\xi}^0)/\delta t\big) \tag{3.3}$$

$$K \delta t \Delta\theta - \theta^0 (s - s^0) + \boldsymbol{B}^d.(\boldsymbol{\xi} - \boldsymbol{\xi}^0) = 0 \tag{3.4}$$

where $s^0 = s(\boldsymbol{\varepsilon}^0, \boldsymbol{\xi}^0, \theta^0)$. A major drawback of this scheme is that the existence of a solution to (3) is not guaranteed. Let us develop this point: if θ is known, then the purely mechanical finite-step problem (3.1-3) has a solution. Similarly, if $(\boldsymbol{u}, \boldsymbol{\xi})$ is fixed, then the thermal problem (3.4) also has a solution. However, one cannot ensure the existence of a solution $(\boldsymbol{u}, \boldsymbol{\sigma}, \theta)$ to the *coupled* thermomechanical problem (3.1-4). This is intimately connected to the non-existence of a variational formulation corresponding to (3).

Such difficulties can be avoided by using the following finite time-step problem:

$$(\boldsymbol{u}, \boldsymbol{\xi}, \theta) \text{ verifies (1.1)-(1.4) at } t^0 + \delta t \tag{4.1}$$

$$\boldsymbol{B} = \boldsymbol{B}^r + \frac{\theta}{\theta^0} \boldsymbol{B}^d \tag{4.2}$$

$$\boldsymbol{B}^r \in \partial I_\mathcal{T}(\boldsymbol{\xi}) \ , \ \boldsymbol{B}^d \in \partial \phi\big((\boldsymbol{\xi} - \boldsymbol{\xi}^0)/\delta t\big) \tag{4.3}$$

$$K \delta t [\Delta\theta + \frac{\nabla\theta^0}{\theta^0}.\nabla(\theta^0 - \theta)] - \theta^0 (s - s^0) + \boldsymbol{B}^d.(\boldsymbol{\xi} - \boldsymbol{\xi}^0) = 0 \tag{4.4}$$

It can be verified that - just as the more intuitive scheme (3) - the incremental problem (4) is a consistent time-discretization of (1), in the sense that (3) coincides with (1) in the limit $\delta t \to 0$ [3, 4]. Motivation of the scheme (3) is that a variational formulation can be given, allowing one to study the existence of solutions. More precisely, it can be proved that solutions of (3) are solutions of the following variational problem

$$\begin{array}{c} find\ (\boldsymbol{u},\boldsymbol{\xi},\theta) \in \mathcal{K}_u \times \mathcal{K}_\xi \times \mathcal{K}_\theta\ such\ that\ for\ all\ (\boldsymbol{u}^*,\boldsymbol{\xi}^*,\theta^*) \in \mathcal{K}_u \times \mathcal{K}_\xi \times \mathcal{K}_\theta : \\ 0 \leq \partial\mathcal{F}[\boldsymbol{u},\boldsymbol{\xi},\theta].(\boldsymbol{u}^*-\boldsymbol{u},\boldsymbol{\xi}^*-\boldsymbol{\xi},\theta^*-\theta) \end{array} \tag{5}$$

where $\mathcal{F}(\boldsymbol{u},\boldsymbol{\xi},\theta) = \mathcal{F}^e(\boldsymbol{u},\boldsymbol{\xi},\theta) + \mathcal{F}^d(\boldsymbol{\xi},\theta) + \mathcal{F}^\theta(\theta)$ and

$$\begin{aligned} \mathcal{F}^e(\boldsymbol{u},\boldsymbol{\xi},\theta) = \quad & \int_\Omega w(\boldsymbol{\varepsilon}(\boldsymbol{u}),\boldsymbol{\xi},\theta)\,d\omega - \int_\Omega \boldsymbol{f}^d.\boldsymbol{u}\,d\omega - \int_{\Gamma^T} \boldsymbol{T}^d.\boldsymbol{u}\,da \\ \mathcal{F}^d(\boldsymbol{\xi},\theta) = \quad & \delta t \int_\Omega \phi\big(\frac{\theta}{\theta^0}\frac{\boldsymbol{\xi}-\boldsymbol{\xi}^0}{\delta t}\big)\,d\omega \\ \mathcal{F}^\theta(\theta) = \quad & \int_\Omega \theta s^0\,d\omega + \delta t \int_\Omega K(-\frac{1}{2}\frac{1}{\theta^0}\|\nabla\theta\|^2 + (\frac{\|\nabla\theta^0\|}{\theta^0})^2\theta)\,d\omega \\ & -\delta t \int_{\Gamma_q} \frac{q^d}{\theta^0}\theta\,da - K'\frac{\delta t}{2}\int_{\Gamma_r}\frac{(\theta-\theta_R)^2}{\theta^0}\,da \end{aligned} \tag{6}$$

Assume in particular that (i) the free energy w is convex in $(\boldsymbol{u},\boldsymbol{\xi})$ and concave in θ, (ii) the dissipation potential ϕ is positively homogeneous of degree 1 (which corresponds to a rate-independent dissipative behaviour). Note that those assumptions are satisfied by a wide range of SMA models (see Section 3 for some examples). In such a situation, the problem (5) can be rewritten as

$$\max_{\theta\in\mathcal{K}_\theta} J(\theta) \tag{7}$$

where

$$J(\theta) = \mathcal{F}^\theta(\theta) + \min_{(\boldsymbol{u},\boldsymbol{\xi})\in\mathcal{K}_u\times\mathcal{K}_\xi} \{\mathcal{F}^e(\boldsymbol{u},\boldsymbol{\xi},\theta) + \mathcal{F}^d(\boldsymbol{\xi},\theta)\} \tag{8}$$

Moreover, the maximization problem (7) admits some solutions (provided adequate functional spaces are chosen for $\mathcal{K}_u$, $\mathcal{K}_\xi$, $\mathcal{K}_\theta$), which ensure existence of solutions to the thermomechanical incremental problem (4) .

2.2 A maximization approach

To solve a problem such as (3) or (4), a general strategy is to solve directly the local equations using a Newton-Raphson algorithm. In such a framework, a partitioning approach is often used: the mechanical and the thermal subproblems are decoupled and solved successively until convergence. The global convergence of such methods is not ensured, and in practice one can face difficulties of convergence when for instance the initial guess is not close enough to the solution. Observe that, in the case of (4), such strategies ignore the variational nature of the problem at hand. As an alternative, using

the variational formulation of the problem, the solution of (4) can notably be found by solving the maximisation problem (7). A lot of well-known methods can be used to solve such a problem, some of them being built-in functions of scientific calculation softwares. Such methods (such as BFGS for instance) are iterative and require the computation of J and its gradient J' (or at least of an ascend direction). In this regard, note from (8) that the calculation of $J(\theta)$ amounts to solve the minimization problem

$$\min_{(\boldsymbol{u},\boldsymbol{\xi})\in\mathcal{K}_u\times\mathcal{K}_\xi} \mathcal{F}^e(\boldsymbol{u},\boldsymbol{\xi},\theta)+\mathcal{F}^d(\boldsymbol{\xi},\theta) \tag{9}$$

for which the local equations (expressing the stationarity of the functional) read as

$$\begin{gathered} \boldsymbol{u}\in\mathcal{K}_u\ ,\boldsymbol{\sigma}\in\mathcal{K}_\sigma\ ,\ \boldsymbol{\xi}\in\mathcal{K}_\xi \\ \boldsymbol{B}^d\in\frac{\theta}{\theta^0}\partial\phi(\frac{\boldsymbol{\xi}-\boldsymbol{\xi}^0}{\delta t})\ ,\ \boldsymbol{B}^r\in\partial I_{\mathcal{T}}(\boldsymbol{\xi}) \\ \boldsymbol{\sigma}=\frac{\partial w}{\partial\boldsymbol{\varepsilon}}\ ,\ \boldsymbol{B}=-\frac{\partial w}{\partial\boldsymbol{\xi}} \\ \boldsymbol{B}=\boldsymbol{B}^d+\boldsymbol{B}^r \end{gathered} \tag{10}$$

Those equations correspond to the backwards Euler scheme for an isothermal problem, with a dissipation potential set equal to $(\theta/\theta_0)\phi$. The calculation of $J(\theta)$ is thus equivalent to solving a incremental problem at a fixed temperature field. It can be proved that the calculation of the gradient $J'(\theta)$ is equivalent to solving a linear thermal problem. As a conclusion, using the variational framework described so far, the solution of the thermomechanical incremental problem can be obtained by solving a sequence of mechanical problems at a fixed temperature field (for evaluating $J(\theta)$) and linear scalar problems (for evaluating $J'(\theta)$). Therefore, that methods allows for a simple implementation of the thermomechanical problem, provided a solver for the isothermal problem is available. That last point is the focus of the next section.

3 CASE OF MICROMECHANICAL SMA MODELS

3.1 Micromechanical modelling

In most of micromechanical models of monocrystalline shape memory alloys, the internal variable $\boldsymbol{\xi}$ is taken as $(\xi_1,\cdots,\xi_n)$ where n is the number of martensitic variants and ξ_i denotes the volume fraction of martensitic variant i. The volume fraction ξ_0 of austenite is given by $\xi_0=1-\sum_{i=1}^n\xi_i$. Since each volume fraction ξ_i $(i=0,\cdots,n)$ must be positive, the variable $\boldsymbol{\xi}$ is required to take values in the convex and closed subset $\mathcal{T}$ of $\mathbb{R}^n$ defined as

$$\mathcal{T}=\{\boldsymbol{\xi}\in\mathbb{R}^n|\xi_i\geq 0\ \forall i;\boldsymbol{\xi}.\mathbf{1}_n\leq 1\} \tag{11}$$

where $\mathbf{1}_n$ is the vector of $\mathbb{R}^n$ with all its components equal to 1. Most of micromechanical SMA models are based on free energy functions of the form

$$w(\boldsymbol{\varepsilon},\boldsymbol{\xi},\theta)=\sum_{i=0}^n\xi_i w_i(\boldsymbol{\varepsilon},\theta)+h^{mix}(\boldsymbol{\xi}) \tag{12}$$

where $w_0(\boldsymbol{\varepsilon}, \theta) = (1/2)\boldsymbol{\varepsilon} : \boldsymbol{L} : \boldsymbol{\varepsilon}$ is the free energy of the austenite (with $\boldsymbol{L}$ symmetric positive definite) and

$$w_i(\boldsymbol{\varepsilon}, \theta) = \frac{1}{2}(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_i^{tr}) : \boldsymbol{L} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_i^{tr}) + c(1 - \log\frac{\theta}{\theta_0}) + \lambda_T \frac{(\theta - \theta_T)}{\theta_T} \tag{13}$$

is the free energy of the martensitic variant i. In (13), $\boldsymbol{\varepsilon}_i^{tr}$ is the transformation strain of martensitic variant i, c is the heat capacity, θ_T is the transformation temperature, and λ_T is the latent heat of the austenite $\rightarrow$ martensite transformation at temperature θ_T. The term h^{mix} in (12) is the interaction energy between the different variants. In the following, we will consider interaction energy h^{mix} of the form

$$h^{mix}(\boldsymbol{\xi}) = \frac{1}{2}(\underline{\boldsymbol{\varepsilon}}^{tr}.\boldsymbol{\xi}) : \boldsymbol{L} : (\underline{\boldsymbol{\varepsilon}}^{tr}.\boldsymbol{\xi}) + (\boldsymbol{J} - \boldsymbol{J}^{tr}).\boldsymbol{\xi} + \frac{1}{2}\boldsymbol{\xi}.\boldsymbol{H}.\boldsymbol{\xi} \tag{14}$$

where $\boldsymbol{H} \in \mathbb{R}^{n\times n}$ is symmetric positive and $\boldsymbol{J}$ is a given vector of $\mathbb{R}^n$. In such case, w is convex in $(\boldsymbol{u}, \boldsymbol{\xi})$. Functions of the form (14) have notably been used in [5, 6] with $\boldsymbol{H}$ and $\boldsymbol{J}$ equal to 0, in which case the obtained expression of w can be proved to be a rigorous lower bound on the effective free energy that would be obtained from relaxation [5, 7]. Concerning the dissipation potential, a classical choice, directly inspired from crystalline plasticity, is to take ϕ as

$$\phi(\dot{\boldsymbol{\xi}}) = \boldsymbol{G}^+.\langle\dot{\boldsymbol{\xi}}\rangle_+ + \boldsymbol{G}^-.\langle\dot{\boldsymbol{\xi}}\rangle_- \tag{15}$$

where $\langle\boldsymbol{x}\rangle_+$ is the positive vector whose component i is $\max(0, x_i)$. Similarly, for any vector $\boldsymbol{x}$, $\langle\boldsymbol{x}\rangle_-$ is the positive vector with components $\max(0, -x_i)$. In (15), $\boldsymbol{G}^+$ and $\boldsymbol{G}^-$ are two given positive vectors of $\mathbb{R}^n$.

3.2 Space discretization

In the following, we discuss the implementation of the general approach presented in Section 2 for the class of micromechanical SMA models introduced in the preceeding subsection. We focus on the problem (9), for which the temperature field θ is fixed. As explained in Section 2, that purely mechanical problem is indeed the central building block for solving the thermomechanical incremental problem.

The problem (9) is solved by a Galerking approach, i.e. (9) is replaced by

$$\min_{(\boldsymbol{u},\boldsymbol{\xi})\in\tilde{\mathcal{K}}_u\times\tilde{\mathcal{K}}_\xi} \mathcal{F}^e(\boldsymbol{u}, \boldsymbol{\xi}, \theta) + \mathcal{F}^d(\boldsymbol{\xi}, \theta) \tag{16}$$

where $\tilde{\mathcal{K}}_u$ and $\tilde{\mathcal{K}}_\xi$ are finite-dimensional subsets of $\mathcal{K}_u$ and $\mathcal{K}_\xi$, respectively. Any $\boldsymbol{u} \in \tilde{\mathcal{K}}_u$ admits a representation of the form

$$\boldsymbol{u}(\boldsymbol{x}) = \boldsymbol{M}_u(\boldsymbol{x}).\underline{\boldsymbol{v}} \tag{17}$$

where $\underline{\boldsymbol{v}} \in \mathbb{R}^M$ and $\boldsymbol{M}_u : \Omega \mapsto \mathbb{R}^{3\times M}$ is a given function. The vector $\underline{\boldsymbol{v}}$ would typically correspond to the nodal displacement vector if the finite element method is used. The

admissibility conditions $\boldsymbol{u} = \boldsymbol{u}^d$ on Γ_u might set restrictions on the admissible values of the vector $\underline{\boldsymbol{v}}$. However, to simplify the presentation, we assume that $\boldsymbol{u}^d = 0$, so that the vector $\underline{\boldsymbol{v}}$ can be considered as free from any constraint. Concerning the space discretization of $\boldsymbol{\xi}$, we assume here that functions in $\tilde{\mathcal{K}}_\xi$ are piecewise constant. More precisely, we assume the existence of a decomposition $\Omega = \bigcup_{i=1}^N \Omega_i$ such that any $\boldsymbol{\xi} \in \tilde{\mathcal{K}}_\xi$ takes a constant value (denoted by $\boldsymbol{\xi}_i$) on Ω_i. In such case, functions $\boldsymbol{\xi}$ in $\tilde{\mathcal{K}}_\xi$ can be written as

$$\boldsymbol{\xi}(\boldsymbol{x}) = \sum_{i=1}^{N} \chi_i(\boldsymbol{x}) \boldsymbol{\xi}_i \tag{18}$$

where χ_i is the characteristic function of Ω_i and $\boldsymbol{\xi}_i \in \mathcal{T}$. The vector $(\boldsymbol{\xi}_1, \cdots, \boldsymbol{\xi}_N)$ is denoted by $\underline{\boldsymbol{\xi}}$.

Substituting (17) and (18) in the expression of $\mathcal{F}^e + \mathcal{F}^d$, the problem (16) takes the form

$$\min_{\underline{\boldsymbol{v}} \in \mathbb{R}^M, \underline{\boldsymbol{\xi}} \in \mathcal{T}^N} \frac{1}{2} \underline{\boldsymbol{v}}.\mathbb{K}.\underline{\boldsymbol{v}} + \frac{1}{2} \underline{\boldsymbol{\xi}}.\mathbb{B}.\underline{\boldsymbol{\xi}} - \underline{\boldsymbol{v}}.\mathbb{C}.\underline{\boldsymbol{\xi}} - \underline{\boldsymbol{v}}.\boldsymbol{F}_u + \underline{\boldsymbol{\xi}}.\boldsymbol{F}_\xi + \Phi(\underline{\boldsymbol{\xi}} - \underline{\boldsymbol{\xi}}^0) \tag{19}$$

where the matrices $\mathbb{K}$ and $\mathbb{B}$ are both symmetric positive definite, the former corresponding to the standard stiffness matrix (see [10] for more details). The function Φ that appears in (19) is the convex function defined by

$$\Phi(\underline{\boldsymbol{\xi}}) = \int_\Omega \frac{\theta}{\theta^0} \phi(\sum_{i=1}^{N} \chi_i(\boldsymbol{x}) \boldsymbol{\xi}_i) d\omega = \sum_{i=1}^{N} p_i \phi(\boldsymbol{\xi}_i) \text{ with } p_i = \int_{\Omega_i} \frac{\theta}{\theta^0} \, d\omega \tag{20}$$

The function in (19) being quadratic with respect to $\boldsymbol{v}$, the minimization with respect to $\boldsymbol{v}$ in (19) can be performed in closed form. The problem (19) is found to reduce to

$$\min_{\underline{\boldsymbol{\xi}} \in \mathcal{T}^N} \frac{1}{2} \underline{\boldsymbol{\xi}}.\mathbb{K}'.\underline{\boldsymbol{\xi}} - \underline{\boldsymbol{\xi}}.\boldsymbol{F}' + \Phi(\underline{\boldsymbol{\xi}} - \underline{\boldsymbol{\xi}}^0) \tag{21}$$

with

$$\mathbb{K}' = \mathbb{B} - \mathbb{C}^T.\mathbb{K}^{-1}.\mathbb{C} \ , \ \boldsymbol{F}' = \mathbb{C}^T.\mathbb{K}^{-1}.\boldsymbol{F}_u + \boldsymbol{F}_\xi \tag{22}$$

It can be verified that the symmetric matrix $\mathbb{K}'$ is positive [10]. Consequently, the function to minimize in (21) is convex (but not quadratic) with respect to $\underline{\boldsymbol{\xi}}$. Using standard results from convex analysis [1], the problem (19) can be rewritten as

$$-\mathbb{K}' \left\{ \begin{array}{c} \boldsymbol{\xi}_1 \\ \vdots \\ \boldsymbol{\xi}_N \end{array} \right\} + \boldsymbol{F}' = \left\{ \begin{array}{c} \boldsymbol{B}_1^r \\ \vdots \\ \boldsymbol{B}_N^r \end{array} \right\} + \left\{ \begin{array}{c} \boldsymbol{B}_1^d \\ \vdots \\ \boldsymbol{B}_N^d \end{array} \right\} \tag{23}$$

$$\boldsymbol{\xi}_i \in \mathcal{T} \ , \boldsymbol{B}_i^r \in \partial I_{\mathcal{T}}(\boldsymbol{\xi}_i) \ , \ \boldsymbol{B}_i^d \in p_i \partial \phi(\boldsymbol{\xi}_i - \boldsymbol{\xi}_i^0) \text{ for } i = 1, \cdots, N$$

The issue of practically solving that problem is the focus of the next subsection.

3.3 Formulation of a linear complementarity problem

The identity matrix of $\mathbb{R}^{n\times n}$ is denoted by $\mathbb{I}_n$, and $\mathbb{E}$ denotes the $nN \times N$ matrix with the following block structure

$$\mathbb{E} = \begin{pmatrix} \mathbf{1}_n & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \ddots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{1}_n \end{pmatrix} \tag{24}$$

For latter reference, we also introduce the two vectors $\tilde{\boldsymbol{G}}^+$ and $\tilde{\boldsymbol{G}}^-$ of $\mathbb{R}^{nN}$ defined by

$$\tilde{\boldsymbol{G}}^+ = \left\{ \begin{array}{c} p_1\boldsymbol{G}^+ \\ \vdots \\ p_N\boldsymbol{G}^+ \end{array} \right\} \ , \ \tilde{\boldsymbol{G}}^- = \left\{ \begin{array}{c} p_1\boldsymbol{G}^- \\ \vdots \\ p_N\boldsymbol{G}^- \end{array} \right\} \tag{25}$$

Consider now a solution $(\boldsymbol{\xi}_j, \boldsymbol{B}^r_j, \boldsymbol{B}^d_j)_{1\leq j\leq N}$ of (23) and define

$$\begin{array}{l} \boldsymbol{\alpha}^+_j = p_j\boldsymbol{G}^+ - \boldsymbol{B}^d_j \quad , \quad \boldsymbol{\mu}^+_j = \langle \boldsymbol{\xi}_j - \boldsymbol{\xi}^0_j \rangle_+ \\ \boldsymbol{\alpha}^-_j = p_j\boldsymbol{G}^- + \boldsymbol{B}^d_j \quad , \quad \boldsymbol{\mu}^-_j = \langle \boldsymbol{\xi}_j - \boldsymbol{\xi}^0_j \rangle_- \\ \gamma_j = 1 - \mathbf{1}_n.\boldsymbol{\xi}_j \end{array} \tag{26}$$

Since $\mathcal{T}$ takes the form (11) and $\boldsymbol{B}^r_j \in \partial I_{\mathcal{T}}(\boldsymbol{\xi}_j)$, there exists $z_j \in \mathbb{R}$ and $\boldsymbol{a}_j \in \mathbb{R}^n$ [10] such that

$$\boldsymbol{B}^r_j = z_j\mathbf{1}_n - \boldsymbol{a}_j \ , z_j \geq 0 \ , \ \boldsymbol{a}_j \geq 0 \ , \ \boldsymbol{a}_j.\boldsymbol{\xi}_j = z_j(1 - \boldsymbol{\xi}_j.\mathbf{1}_n) = 0 \tag{27}$$

Define

$$\boldsymbol{\alpha}^\pm = \left(\begin{array}{c} \boldsymbol{\alpha}^\pm_1 \\ \vdots \\ \boldsymbol{\alpha}^\pm_N \end{array} \right) \ , \ \boldsymbol{\mu}^\pm = \left(\begin{array}{c} \boldsymbol{\mu}^\pm_1 \\ \vdots \\ \boldsymbol{\mu}^\pm_N \end{array} \right) \ , \ \boldsymbol{a} = \left(\begin{array}{c} \boldsymbol{a}_1 \\ \vdots \\ \boldsymbol{a}_N \end{array} \right) \ , \ \boldsymbol{\gamma} = \left(\begin{array}{c} \gamma_1 \\ \vdots \\ \gamma_N \end{array} \right) \ , \ \boldsymbol{z} = \left(\begin{array}{c} z_1 \\ \vdots \\ z_N \end{array} \right) \tag{28}$$

Setting $k = (3n + 1)$, we consider the two following vectors of $\mathbb{R}^k$:

$$\boldsymbol{s} = \left(\begin{array}{c} \boldsymbol{\alpha}^+ \\ \boldsymbol{\alpha}^- \\ \underline{\boldsymbol{\xi}} \\ \boldsymbol{\gamma} \end{array} \right) \ , \ \boldsymbol{x} = \left(\begin{array}{c} \boldsymbol{\mu}^+ \\ \boldsymbol{\mu}^- \\ \boldsymbol{a} \\ \boldsymbol{z} \end{array} \right) \tag{29}$$

Using the relations (23), it can be verified that $(\boldsymbol{x}, \boldsymbol{s})$ are solution of the problem

$$\textit{Find } \boldsymbol{x} \in \mathbb{R}^k \textit{ and } \boldsymbol{s} \in \mathbb{R}^k \textit{ such that } \boldsymbol{s} = \mathbb{M}.\boldsymbol{x} + \boldsymbol{q} \ , \ \boldsymbol{s} \geq 0 \ , \ \boldsymbol{x} \geq 0, \boldsymbol{s}.\boldsymbol{x} = 0 \tag{30}$$

where $\mathbb{M} \in \mathbb{R}^{k\times k}$ and $\boldsymbol{q} \in \mathbb{R}^k$ are defined by

$$\mathbb{M} = \begin{pmatrix} \mathbb{K}' & -\mathbb{K}' & -\mathbb{I}_{nN} & \mathbb{E} \\ -\mathbb{K}' & \mathbb{K}' & \mathbb{I}_{nN} & -\mathbb{E} \\ \mathbb{I}_{nN} & -\mathbb{I}_{nN} & \mathbf{0} & \mathbf{0} \\ -\mathbb{E}^T & \mathbb{E}^T & \mathbf{0} & \mathbf{0} \end{pmatrix} \ , \ \boldsymbol{q} = \begin{pmatrix} \tilde{\boldsymbol{G}}^+ - \boldsymbol{F}' + \mathbb{K}'.\underline{\boldsymbol{\xi}^0} \\ \tilde{\boldsymbol{G}}^- + \boldsymbol{F}' - \mathbb{K}'.\underline{\boldsymbol{\xi}^0} \\ \underline{\boldsymbol{\xi}^0} \\ \mathbf{1}_N - \mathbb{E}^T.\underline{\boldsymbol{\xi}^0} \end{pmatrix} \tag{31}$$

Conversely, it can easily be verified that any solution of (30) generates a solution of the incremental problem (23), so that the two problems (23) and (30) are equivalent. The motivation of that reformulation is that (30) is a standard problem in mathematical programming. It is known as a Linear Complementarity Problem (LCP) and has been extensively studied [8, 9]. In particular, efficient numerical algorithms, such as interior-point methods, have been developed and are now available in various toolboxes. That reformulation thus allows for an easy and efficient way of solving the incremental problem, building on existing algorithms suited to large-scale problems. Is should be mentionned that solving a LCP amounts to solve a quadratic minimization problem (with linear constraints). As a consequence, the change of variables (26) allows us to turn the convex but non quadratic problem (23) into an equivalent quadratic problem, easier to solve. Some examples of numerical simulations are presented in [10].

It would be interesting to study if the proposed method could be extended to more sophisticated micromechanical models, in order to account for crystalline texture [7] or large strain effects [11].

REFERENCES

[1] Brézis, H. *Opérateurs maximum monotones et semigroupes de contractions dans les espaces de Hilbert*. North-Holland, Amsterdam, (1972).

[2] Peigney, M., Shakedown theorems and asymptotic behaviour of solids in non-smooth mechanics. *Eur.J.Mechanics A* (2010) **29**:785-793.

[3] Yang, Q., Stainier, L. and Ortiz, M., A variational formulation of the coupled thermo-mechanical boundary-value problem for general dissipative solids. *J. Mech. Phys. Solids* (2006) **54**:401-424.

[4] Peigney, M., A time-integration scheme for thermomechanical evolutions of shape-memory alloys. *C.R.Mécanique* (2006) **334**:266-271.

[5] Govindjee, S. and Miehe, C., A multi-variant martensitic phase transformation model : formulation and numerical implementation. *Comput. Mech. Appli. Mech. Eng.* (2001) **191**:215-238.

[6] Anand, L. and Gurtin, M.E., Thermal effects in the superelasticity of crystalline shape-memory materials. *J. Mech. Phys. Solids* (2003) **51**:1015-1058.

[7] Peigney, M., A non-convex lower bound on the effective free energy of polycrystalline shape memory alloys. *J. Mech. Phys. Solids* (2009) **57**:970-986.

[8] Ye, Y. *Interior Point Algorithms : theory and analysis*. Wiley Interscience (1997).

[9] Wright, S.J. *Primal-dual interior-point methods*. Society for Industrial and Applied Mathematics (1997).

[10] Peigney, M., Seguin, J.P. and Herve-Luanco, E., Numerical simulation of shape memory alloys structures using interior-point methods. *Int.J.Sol.Struct.* (2011) doi:10.1016/j.ijsolstr.2011.05.017.

[11] Peigney, M., Recoverable strains in composite shape memory alloys. *J. Mech. Phys. Solids* (2008) **56**:360-275.