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A robust and efficient radial return algorithm based on incremental energy minimization for the 3D Souza-Auricchio model for shape memory alloys

Giulia Scalet [a], [b], [*], Michaël Peigney [c]

[a] Department of Civil Engineering and Architecture, University of Pavia, via Ferrata 3, 27100 Pavia, Italy
[b] Laboratoire de Mécanique des Solides, Ecole Polytecnique, CNRS, Université Paris-Saclay, 91128 Palaiseau, France
[c] Laboratoire Navier, UMR 8205, Ecole des Ponts, IFSTTAR, CNRS, UPE, Champs-sur-Marne, France

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ABSTRACT

The present paper focuses on the numerical simulation of quasi-static problems involving shape memory alloy (SMA) structures or components. Phenomenological constitutive models formulated within the continuum thermodynamics with internal variable framework describe phase transformation in a SMA by introducing a suitable set of internal variables, which may be constrained to satisfy a set of inequalities. The numerical treatment of such constraints, together with the presence of non-smooth functions and/or complementary conditions in the model formulation, is not an easy task and strongly influences the numerical convergence, algorithm robustness, and computational times. The aim of this paper is to propose a novel state-update procedure for the three-dimensional phenomenological model known as the Souza-Auricchio model. The proposed radial return algorithm, relying on an incremental energy minimization approach, allows for an easy implementation of model equations and internal constraints and avoids the use of regularization parameters for the treatment of non-smooth functions. Several numerical simulations assess the noticeable efficiency, robustness, and performance of the proposed approach, while comparisons with a classical algorithm proposed in the literature show the reduced computational times.

1. Introduction

Shape memory alloys (SMAs) are smart materials with the ability to recover large strains after thermal cycling or mechanical loading/unloading (Lagoudas, 2008). Thanks to these unique properties, denoted as *shape memory effect* and *pseudoelasticity*, SMA materials are employed in numerous commercial applications, ranging from the biomedical, aerospace, automotive, and earthquake engineering fields to recent technologies as additive manufacturing and active textiles (Jani et al., 2014).

Motivated by the ever-increasing use of SMA-based components and devices, a lot of research has been dedicated to the modeling, simulation, and experimental testing of these alloys.

Several constitutive models have been proposed in the literature for describing the complex behavior of SMAs; generally, they are categorized in macroscopic, microscopic, and micro-macro models. A description of all the modeling approaches is out of the present scope; the reader is referred to Cisse et al. (2016) for a recent review on the topic. Among the others, phenomenological macroscopic models formulated within the framework of continuum thermodynamics with internal variables attract large engineering interest. Starting from pioneering models involving only scalar internal variables (Tanaka and Nagaki, 1982), such models have actually reached high levels of accuracy and refinement (Auricchio et al., 2014a; Lagoudas et al., 2012; Zaki and Moumni, 2007). Most of the models are in fact able to describe several mechanisms and effects characterizing SMA behavior, e.g., martensite reorientation (Arghavani et al., 2010; Pan et al., 2007; Popov and Lagoudas, 2007), twinned-detwinned martensites (Auricchio and Bonetti, 2013), thermomechanical coupling (Auricchio et al., 2016), R-phase and anisotropy (Sedlák et al., 2012), asymmetric behavior in tension and compression (Auricchio et al., 2009b), transformation-induced plasticity (Hartl and Lagoudas, 2009; Auricchio et al., 2007),

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[*] Corresponding author. Department of Civil Engineering and Architecture, University of Pavia, via Ferrata 3, 27100 Pavia, Italy.
E-mail address: giulia.scalet@unipv.it (G. Scalet).

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viscoplasticity (Chemisky et al., 2014), internal damage (Hartl et al., 2014), functional fatigue effects (Barrera et al., 2014), microstructure-dependent inelasticity (Grandi and Stefanelli, 2014), and the two-way shape memory effect (Lexcellent et al., 2000).

One of the major concerns associated to constitutive modeling is the need of suitable numerical algorithms to treat non-smooth functions and/or local constraints deriving from the set of nonlinear constitutive equations describing material behavior. The presence of equality/inequality constraints in the evolution problem and/or on internal variables as well as the introduction of non-smooth functions in the model definition, often treated through regularized terms, may prevent numerical convergence and may influence numerical robustness, accuracy, and computational times. Therefore, a robust and accurate numerical implementation is of extreme importance for the design of novel structures (Peraza-Hernandez et al., 2013) and for the development of novel technologies (Meisel et al., 2015). The implementation generally consists, first, in the time-integration of the system of constitutive equations and, then, in a state-update procedure to derive the updated variables.

Several models are available in a suitable form to perform simulations of complex SMA-based geometries subjected to general thermomechanical loading paths in both finite element (Arghavani et al., 2010; Sedlák et al., 2012; Zaki, 2012) and isogeometric analysis (Auricchio et al., 2015; Dhote et al., 2015) frameworks. The state-update procedures generally adopted to treat SMA constitutive equations are based on return-map schemes, incremental energy minimization approaches, or algorithms for mathematical programming.

A wide class of SMA models implements a return-map-like procedure in an implicit framework (Auricchio and Petrini, 2004; Qidwai and Lagoudas, 2000; Lagoudas et al., 2012; Zaki, 2012; Hartl and Lagoudas, 2009), even if some works have recently proposed implementations in an explicit environment (Stebner and Brinson, 2013; Scalet et al., 2015). The work by Popov and Lagoudas (2007) applies an extension of the closest-point projection algorithm to treat a SMA model incorporating single- and multi-variant martensites. The advantage in using such a procedure is granted by its good numerical performance and well-established numerical properties.

To eliminate the need for a predictor-corrector-type scheme and to omit an active set search, which may become elaborate in the presence of coupled evolution equations and internal constraints, Kiefer et al. (2012) presented two alternative algorithms for the integration of the constitutive equations for magnetic SMAs, namely, the classical return-map scheme and a Fischer-Burmeister-based algorithm. The work demonstrates a greater numerical efficiency of the Fischer-Burmeister-based algorithm, compared to the classical return-mapping. In the context of SMA micromechanical modeling, it is noteworthy to cite the contributions by Bartel and Hackl (2009, 2010); Bartel et al. (2011), who also employed the Fischer-Burmeister complementary function. Recently, Auricchio et al. (2014a) have proposed the use of the Fischer-Burmeister function to treat the inequality constraints on the internal variables and the Kuhn-Tucker complementary inequality conditions deriving from a plasticity-like model formulation. A regularized Fischer-Burmeister function is adopted to treat the non-differentiability of the function when both the arguments are equal to zero.

An alternative approach to return-map procedures is the class of variational methods, which relies on an incremental energy minimization approach. Sedlák et al. (2012) applied the Nelder-Mead minimization algorithm to solve the derived problem for SMAs and introduced a regularization energy to assure the fulfillment of constraints on internal variables. Stupkiewicz and Petryk (2013) presented a pseudoelastic model within the incremental energy minimization framework and proposed an unified augmented Lagrangian treatment of both constitutive constraints and non-smooth dissipation function.

Another approach consists in rewriting the problem as a mathematical programming problem which is solved using general optimization methods. Peigney et al. (2011) applied an incremental variational approach to SMAs and reformulated the incremental problem as a linear complementarity problem. The advantage of the formulation is to solve simultaneously the equilibrium equations and the constitutive laws, taking the internal constraints into account. The obtained formulation leads to a simple and efficient numerical algorithm, solved using interior-point methods.

In the present paper, we focus on the three-dimensional phenomenological model introduced by Souza et al. (1998), and then treated and generalized in Auricchio and Petrini (2004); Evangelista et al. (2009) (hence the denomination *Souza-Auricchio model*, in the following). The model has received a large attention thanks to several advantageous features (Grandi and Stefanelli, 2015), such as a simple plasticity-like formulation, few parameters, and a robust numerical implementation, which have allowed its application to the simulation of a wide range of devices (Auricchio et al., 2014b). Several works focused on the numerical implementation of this model, to treat the evolution of the tensorial internal variable (i.e., the transformation strain), subjected to a saturation constraint. Souza et al. (1998) adopted a return-map scheme and used a criterion for the nucleation of the product phase, while Auricchio and Petrini (2004) used a regularized parameter to treat the case of vanishing transformation strain and Jähne (2012) proposed an explicit integration scheme. Recently, Artioli and Bisegna (2015) have adopted an incremental energy minimization approach for the solution of the constitutive equations, without introducing any regularization, and have shown the effect of the regularized term on material response. The use of a regularization parameter strongly influences the predicted response at the cost of accuracy. Arghavani et al. (2011b) proposed an integration algorithm for a finite-strain extension of the Souza-Auricchio model, based on a logarithmic mapping and a nucleation-completion criterion, while Arghavani et al. (2011a) proposed an improved alternative constitutive model for a finite-strain extension of the Souza-Auricchio model, expressed in terms of only symmetric tensors.

The present paper aims to propose a novel solution algorithm for the Souza-Auricchio model. Among the several numerical approaches cited above, the proposed algorithm belongs to the class of variational methods relying on an incremental energy minimization approach. The evolution of the transformation strain in a finite time step incrementally minimizes a convex functional, given by the sum of the elastic energy and the dissipation function. The treatment is then based on a radial-return algorithm and a standard Newton-Raphson scheme is adopted to solve the single scalar equation in both the unsaturated and saturated phase transformation cases. The solution algorithm as well as the initial guess for the resultant nonlinear equation are also discussed. The formulation is here restricted to the framework of infinitesimal strain theory; however, the present approach can be applied to geometric nonlinear problems.

The choice of using this approach is due to its suitable variational structure which facilitates the treatment of internal constraints and allows for an efficient numerical implementation. The advantages of the proposed algorithm are its equation simplicity, easy implementation, the possibility of avoiding regularized terms in both energy/dissipation definition and transformation strain norm, and, overall, the reduced computational times. The actual