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SPACE-TIME ERROR BOUNDS FOR AN ISOTHERMAL MODEL FOR SHAPE MEMORY ALLOYS

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Summary. We present some error estimates for space-time discretizations of a three-dimensional model for isothermal stress-induced transformations in shape-memory materials. After recalling some basic modeling frame, a fully-discrete approximation is presented and an explicit space-time convergence rate $h^{\alpha/2}+\tau^{1/2}$ for some $\alpha \in (0,1]$ is derived. The estimates are valid uniformly on the whole time interval and require no extra regularity on solutions.

1 THE MODEL

We shall focus on error control for fully-discrete approximations in the context of solids undergoing stress-induced martensitic transformations. More specifically, we address a phenomenological, small-deformation model for polycrystalline materials describing both the shape memory and the superelastic effect. The model has been originally advanced by Souza, Mamiya, & Zouain [SMZ98] and then combined with finite elements by Auricchio and collaborators [AuP02]. The state of the material is determined by its displacement $\boldsymbol{u} : \Omega \to \mathbb{R}^d$ with respect to the reference configuration $\Omega \subset \mathbb{R}^d$ $(d = 2, 3)$ and by a tensorial internal variable $z : \Omega \to \mathbb{R}^{d\times d}_{\text{dev}}$ (deviatoric d-tensors) which represent the inelastic part of the deformation ε, namely $z = \varepsilon - \mathbf{C}\sigma$ where $\mathbf{C}$ is the elasticity tensor and σ is the stress. In fact, z corresponds to a sort of an *oriented* proportion of detwinned martensites (*product phase*) with respect to twinned martensites and austenite (*parent phase*). The temperature of the specimen is assumed to be fixed throughout.

The free energy density of the material depends on ε only via $\varepsilon_{\text{el}} = \varepsilon - z$:

$$W(\varepsilon, z) = \frac{1}{2}\mathbf{C}(\varepsilon - z):(\varepsilon - z) + H(z) + \frac{\nu}{2}|\nabla z|^2. \tag{1.1}$$

Here, the *hardening function* $H : \mathbb{R}^{d\times d}_{\rm dev} \to \mathbb{R}$ is given by

$$H(z) = c_1\sqrt{\rho^2{+}|z|^2} + \frac{c_2}{2}|z|^2 + \frac{(|z|{-}c_3)_+^4}{\rho(1{+}|z|^2)} \tag{1.2}$$

where the user-defined parameter $\rho > 0$ is small and c_1, c_2, and c_3 are given and represent a superelastic-transformation stress-activation level, a hardening modulus with respect to the internal variable z, and the maximum modulus of transformation strain that can be obtained by alignment (detwinning) of the martensitic variants, respectively.

The constitutive relations are given in the form

$$\sigma = \partial W/\partial\varepsilon = \mathbf{C}(\varepsilon{-}z), \quad \xi = -\delta W/\delta z = \mathbf{C}(\varepsilon{-}z) - \mathrm{D}_z H(z) + \nu\Delta z, \tag{1.3}$$

where ξ denotes the thermodynamic force associated with z. The evolution of the material will be described by the following classical relations:

$$\xi \in R\partial|\dot z|, \qquad \mathrm{div}\sigma + \boldsymbol{f} = \mathbf{0} \ \text{ in } \Omega, \ \ \sigma\boldsymbol{n} = \boldsymbol{T} \ \text{ in } \Gamma_{\rm Neu}, \ \ \boldsymbol{u} = \mathbf{0} \ \text{ in } \Gamma_{\rm Dir} \tag{1.4}$$

where $\boldsymbol{f}$ and $\boldsymbol{T}$ are a given body force and a surface traction, respectively. Here we assume the boundary $\partial\Omega$ to be partitioned in two disjoint open sets $\Gamma_{\rm Neu}$ and $\Gamma_{\rm Dir}$ with $\partial\Gamma_{\rm Neu} = \partial\Gamma_{\rm Dir}$ (in $\partial\Omega$) such that $\Gamma_{\rm Dir}$ has positive surface measure. The flow rule above corresponds to the classical *generalized normality assumption* ($R > 0$ is the fixed *transformation radius*), and the symbol ∂ stands for the subdifferential in the sense of convex analysis.

Our interest in this model is mainly motivated by its ability to describe (at least to a qualitative extent) the thermomechanical behavior of SMAs by means of a small number of easily fitted material parameters (8 material constants in 3D). Another interesting feature of the Souza-Auricchio model is that it turns out to be quite naturally posed in the frame of the variational theory of rate-independent systems. This feature was indeed exploited in [AMS08], where wellposedness issues for continuous problems as well as the convergence of discretizations and regularizations has been discussed. In particular some fully-discrete approximations $(\boldsymbol{u}_{\tau,h}, z_{\tau,h})$ obtained by implicit Euler discretization in time (τ is the fineness of the time-partition) and piecewise linear finite elements in space (h is the mesh size) are proved in [AMS08, Theorem 7.1] to converge to the unique solution of the time-continuous quasistatic evolution problem.

The focus here is to provide explicit convergence rates in space and time for these fully-discrete approximations. In particular, we check that

$$\exists\alpha \in (0,1] \ : \ \|\boldsymbol{u}{-}\boldsymbol{u}_{\tau,h}\|_{\mathrm{H}^1(\Omega;\mathbb{R}^d)} {+} \|z{-}z_{\tau,h}\|_{\mathrm{H}^1(\Omega;\mathbb{R}^{d\times d})} \le O(h^{\alpha/2}{+}\tau^{1/2}).$$

In the special case of a convex polyhedron Ω and homogeneous Dirichlet conditions for the displacement the parameter α can be chosen to be $\alpha = 1$.

The above quantitative control is, to our knowledge, the first result in this direction in the context of the mechanics of solid-solid phase transformations. Note that our error estimate is derived under natural regularity requirements. Namely, it depends solely on data and no extra-smoothness of the solution $(\boldsymbol{u}, z)$ is assumed. This specific feature sets this result apart from the existing literature on error control for time- or space-time discretizations of variational evolution problems (inequalities) arising in elasto-plasticity.

2 SPACE-TIME DISCRETIZATION: MAIN RESULT

Let Ω be a non-empty, bounded, and connected polyhedron in $\mathbb{R}^d$ ($d = 2, 3$). We define $\varepsilon = \varepsilon(\boldsymbol{u}) = \frac{1}{2}(\nabla\boldsymbol{u}+\nabla\boldsymbol{u}^{\mathrm{T}})$, where $\boldsymbol{u}$ is the displacement, and

$$\mathcal{U} \overset{\text{def}}{=} \left\{ \boldsymbol{u} \in \mathrm{H}^1(\Omega;\mathbb{R}^d) \,\middle|\, \boldsymbol{u} = \boldsymbol{0} \text{ on } \Gamma_{\text{Dir}} \right\}, \quad \mathcal{Z} \overset{\text{def}}{=} \mathrm{H}^1(\Omega;\mathbb{R}^{d\times d}_{\text{dev}}), \quad \mathcal{Q} \overset{\text{def}}{=} \mathcal{U} \times \mathcal{Z}.$$

The symbol $\langle\cdot,\cdot\rangle$ denotes the duality pairing between $\mathcal{Q}'$ and $\mathcal{Q}$. We indicate the state variables by $q = (\boldsymbol{u}, z) \in \mathcal{Q}$. As for the loadings $\boldsymbol{f}$ and $\boldsymbol{T}$ in (1.4) we require that $\boldsymbol{\ell}$ defined via

$$\langle \boldsymbol{\ell}(t), q\rangle \overset{\text{def}}{=} \int_\Omega \boldsymbol{f}(t)\cdot\boldsymbol{u}\,\mathrm{d}x + \int_{\Gamma_{\text{Neu}}} \boldsymbol{T}(t)\cdot\boldsymbol{u}\,\mathrm{d}x,$$

satisfies $\boldsymbol{\ell} \in \mathbf{C}^1([0,T];\mathrm{L}^2(\Omega,\mathbb{R}^d\times\mathbb{R}^{d\times d}_{\text{dev}}))$. Furthermore, we choose an initial datum $q_0 = (\boldsymbol{u}_0, z_0) \in \mathcal{S}(0)$ where the set $\mathcal{S}(t)$ of *stable states at time* $t \in [0,T]$ is defined as the set of all $q = (\boldsymbol{u}, z) \in \mathcal{Q}$ satisfying the condition

$$\int_\Omega W(\boldsymbol{u},z)\,\mathrm{d}x - \langle\boldsymbol{\ell}(t),q\rangle \le \int_\Omega W(\boldsymbol{u},z)\,\mathrm{d}x - \langle\boldsymbol{\ell}(t),q\rangle + \int_\Omega R|\widehat{z}-z|\,\mathrm{d}x \tag{2.5}$$

for all $\widehat{q} = (\widehat{\boldsymbol{u}},\widehat{z}) \in \mathcal{Q}$. The variational formulation of the quasi-static evolution problem consists in finding $q : [0,T] \to \mathcal{Q}$ such that

$$q(0) = q_0, \tag{2.6a}$$

$$\int_\Omega \mathbf{C}(\varepsilon(\boldsymbol{u})-z):\varepsilon(\boldsymbol{v})\,\mathrm{d}x = \langle\boldsymbol{\ell},\boldsymbol{v}\rangle \qquad \text{for all } \boldsymbol{v}\in\mathcal{U}, \tag{2.6b}$$

$$\begin{aligned}&\int_\Omega \big((\mathbf{C}(z-\varepsilon(\boldsymbol{u})) + \mathrm{D}_z H(z)):(w-\dot z) + \nu\nabla z:\nabla(w-\dot z)\big)\,\mathrm{d}x \\ &\qquad + \int_\Omega R|w|\,\mathrm{d}x - \int_\Omega R|\dot z|\,\mathrm{d}x \ge 0 \qquad \text{for all } w\in\mathcal{Z},\end{aligned} \tag{2.6c}$$

almost everywhere in time. The following wellposedness theorem is proved in [AMS08].

Theorem 2.1 (Wellposedness)**.** *For each* $q_0 \in \mathcal{S}(0)$ *problem* (2.6) *admits a unique solution* $q : [0,T] \to \mathcal{Q}$*, which even lies in* $\mathbf{C}^{\text{Lip}}([0,T];\mathcal{Q})$*.*

Let us now introduce our space-time discretization of (2.6). To this aim, we choose a sequence $(\Pi_\tau)_{\tau>0}$ of partitions $\{\, 0 = t^0_\tau < t^1_\tau < \cdots < t^{k_\tau}_\tau = T \,\}$ of the time interval $[0,T]$ with $\max\{\, t^k_\tau - t^{k-1}_\tau \,:\, k = 1,...,k_\tau \,\} \le \tau$ and a sequence $(\mathcal{Q}_h)_{h>0}$ of finite-dimensional spaces exhausting $\mathcal{Q}$. In particular, assume to be given a regular triangulation $\{\mathcal{T}_k\}$ of Ω and choose $\mathcal{U}_h$ and $\mathcal{Z}_h$ to be the subspaces of continuous, piecewise polynomials of fixed degree $m \ge 1$ on $\{\mathcal{T}_k\}$. Finally, let $\mathcal{Q}_h \overset{\text{def}}{=} \mathcal{U}_h \times \mathcal{Z}_h$. As for the initial value, we shall ask for $q_{0,h} \in \mathcal{S}_h(0)$ where the set of *approximate stable states* is defined as in (2.5) by replacing $\mathcal{Q}$ by $\mathcal{Q}_h$.

Our space-time discretization of (2.6) consists in finding $q^i_{\tau,h} = (\boldsymbol{u}^i_{\tau,h}, z^i_{\tau,h}) \in \mathcal{Q}_h$ for $i = 0, 1, \ldots, k_\tau$ such that

$$q^0_{\tau,h} = q_{0,h}, \tag{2.7a}$$

$$\int_\Omega \mathbf{C}(\varepsilon(\boldsymbol{u}^i_{\tau,h}) - z^i_{\tau,h}) : \varepsilon(\boldsymbol{v}_h)\,\mathrm{d}x = \langle \boldsymbol{\ell}(t^i_\tau), \boldsymbol{v}_h \rangle \quad \text{for all } \boldsymbol{v}_h \in \mathcal{U}_h, \tag{2.7b}$$

$$\begin{aligned}\int_\Omega \big(\mathbf{C}(z^i_{\tau,h} - \varepsilon(\boldsymbol{u}^i_{\tau,h})) + \mathrm{D}_z H(z^i_{\tau,h}) : (w_h - \delta z^i_{\tau,h}) + \nu \nabla z^i_{\tau,h} : \nabla (w_h - \delta z^i_{\tau,h})\big)\,\mathrm{d}x \\ + \int_\Omega R|w_h|\,\mathrm{d}x - \int_\Omega R|\delta z^i_{\tau,h}|\,\mathrm{d}x \ge 0 \quad \text{for all } w_h \in \mathcal{Z}_h\end{aligned} \tag{2.7c}$$

for $i = 1, \ldots, k_\tau$. Here we used the short-hand notation $\delta z^i_{\tau,h} \overset{\text{def}}{=} (z^i_{\tau,h} - z^{i-1}_{\tau,h})/(t^i_\tau - t^{i-1}_\tau)$. Because of convexity, conditions (2.7b)-(2.7c) are equivalent to solving the corresponding incremental minimization problems.

We shall denote by $q_{\tau,h} = (\boldsymbol{u}_{\tau,h}, z_{\tau,h}) : [0,T] \to \mathcal{Q}_h \subset \mathcal{Q}$ the left-continuous piecewise-constant-in-time interpolants of the above fully-discrete solutions. The above scheme has been proved to be wellposed and convergent in [AMS08]. Here is our main result.

Theorem 2.2 (Error control)**.** *For all $q_0 \in \mathcal{S}(0)$, there exist a sequence $q_{0,h} \in \mathcal{S}_h(0)$ of approximating initial with $q_{0,h} \to q_0$ and unique solutions $q^i_{\tau,h}$ of (2.7). Moreover, there exist $\alpha \in (0,1]$ and $C_{\text{err}} > 0$ (all independent from τ and h) such that*

$$\max_{t \in [0,T]} \|q(t) - q_{\tau,h}(t)\|_{\mathcal{Q}} \le C_{\text{err}}(h^{\alpha/2} + \tau^{1/2}).$$

In case Ω is convex and $\Gamma_{\text{Neu}} = \emptyset$, one can choose $\alpha = 1$.

A proof of this error estimate is reported in [MPP08] in the more general setting of an abstract evolutionary inequality.

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