Error bounds for space-time discretizations of a 3D model for shape-memory materials

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Abstract This paper deals with error estimates for space-time discretizations of a three-dimensional model for isothermal stress-induced transformations in shape-memory materials. After recalling existence and uniqueness results, a fully-discrete approximation is presented and an explicit space-time convergence rate of order $h^{\alpha/2}+\tau^{1/2}$ for some $\alpha\in(0,1]$ is derived, which is valid uniformly on the whole continuous time interval.

1 Introduction

This note is concerned with error control for fully-discrete approximations in the context of solids undergoing martensitic transformations. More specifically, we address the description of the isothermal 3D quasistatic evolution of shape-memory alloys (SMAs). The latter are metallic alloys showing some surprising thermo-mechanical behavior, namely, strongly deformed specimens regain their original shape after a thermal cycle (*shape-memory effect*). Moreover, within some specific (suitably high) temperature range, SMAs are *superelastic*, meaning that they fully

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recover comparably large deformations. These features are not present (at least to this extent) in most materials traditionally used in Engineering and, thus, are at the basis of innovative and commercially valuable applications. Nowadays, SMAs are successfully used in many applications among which biomedical devices (vascular stents, archwires, endo-guidewires) and MEMS (actuators, valves, mini-grippers and positioners).

We will focus on a phenomenological, small-deformation model for polycrystalline materials describing both the shape memory and the superelastic effect. (In the present isothermal reduction shape-memory effect is actually not reproduced, and we refer to [Mie07, MPP08] for models driven by temperature changes.) The model has been originally advanced by SOUZA, MAMIYA, & ZOUAIN [SMZ98] and then combined with finite elements by AURICCHIO and collaborators [AuS01, AuP04]. 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 $z : \Omega \to \mathbb{R}^{d\times d}_{\mathrm{dev}}$ (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*).

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 (7 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 [Mie05]. This feature was indeed exploited in [AMS08], where wellposedness issues for continuous problems (constitutive relation and quasistatic evolution) 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 of this note is to provide explicit convergence rates in space and time for these fully-discrete approximations. In particular, we check that

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

In the special case of a convex polyhedron Ω and homogeneous Dirichlet conditions for the displacement the parameter α can be chosen to be $\alpha = 1$. A more elaborate and general theory will be developed in [MP*08].

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 (see [ACZ99, HaR99]).

Related numerical approaches to rate-independent models for SMA are given in [KMR05, MiR08, MPP08]. However, there the method of Γ-convergence is employed, which guarantees the convergence of subsequences only and provides no quantitative error estimates.

2 The mechanical model

We briefly review the mechanical model, the interested reader being referred to the original papers [SMZ98, AuP02, AuP04, ARS07] for additional details. Let the reference configuration Ω be a non-empty, bounded, and connected polyhedron in $\mathbb{R}^d$ $(d = 2,3)$. We assume the boundary $\partial\Omega$ to be partitioned in two disjoint open sets Γ_{Neu} and Γ_{Dir} with $\partial\Gamma_{\text{Neu}} = \partial\Gamma_{\text{Dir}}$ (in $\partial\Omega$) such that Γ_{Dir} has positive surface measure.

Moving into the frame of Generalized Standard Materials (see e.g., [Mie06] and within the small-strain regime), we additively decompose the linearized deformation $\varepsilon = \varepsilon(\boldsymbol{u}) = \frac{1}{2}(\nabla\boldsymbol{u}+\nabla\boldsymbol{u}^{\mathrm{T}})$, where $\boldsymbol{u}$ is the displacement, into the elastic part $\varepsilon_{\text{el}} \in \mathbb{R}^{d\times d}_{\text{sym}}$ and the inelastic (or transformation) part $z \in \mathbb{R}^{d\times d}_{\text{dev}}$. The free energy density of the material depends on ε only via $\varepsilon_{\text{el}} = \varepsilon - z$:

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

Here, $\mathbf{C}$ is a positive definite elasticity tensor (for isotropic materials, for simplicity), $\nu > 0$ is expected to measure some nonlocal interaction effect for the internal variable z, and ∇z stands for the usual gradient with respect to spatial variables. Indeed, gradients of inelastic strains have already been considered in the frame of shape-memory materials by FRÉMOND [Fré02] and the reader is referred also to ARNDT ET AL. [AGR03], FRIED & GURTIN [FrG94], MIELKE & ROUBÍČEK [MiR03] for examples and discussions on nonlocal energy contributions. Finally, the *hardening function* $H : \mathbb{R}^{d\times d}_{\text{dev}} \to \mathbb{R}$ is given by

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

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. One has to mention that this specific form of W can be much generalized and is here fixed for definiteness only. In particular, W is a ρ-approximation of the original choice of [SMZ98] which in turn corresponds to the limit $(\rho,\nu) \to (0,0)$ (see [AMS08]).

The constitutive relations are given in the form

$$\sigma = \partial W/\partial \varepsilon = \mathbf{C}(\varepsilon - z), \tag{3a}$$
$$\xi = -\delta W/\delta z = \mathbf{C}(\varepsilon - z) - \mathrm{D}_z H(z) + \nu \Delta z, \tag{3b}$$

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

$$\xi \in R\partial|\dot{z}|, \tag{3c}$$
$$\mathrm{div}\sigma + \boldsymbol{f} = \mathbf{0} \text{ in } \Omega, \;\; \sigma\boldsymbol{n} = \boldsymbol{T} \text{ in } \Gamma_{\mathrm{Neu}}, \;\; \boldsymbol{u} = \mathbf{0} \text{ in } \Gamma_{\mathrm{Dir}}, \tag{3d}$$

The latter equation gives the equilibrium equations, where $\boldsymbol{f}$ and $\boldsymbol{T}$ are a given body force and a surface tension, respectively. The flow rule (3c) 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, viz.,

$$\xi \in R\partial|\dot{z}| \quad \text{if and only if} \quad \xi{:}(w - \dot{z}) + R|w| - R|\dot{z}| \leq 0 \text{ for all } w \in \mathbb{R}^{d\times d}_{\mathrm{dev}}.$$

3 The variational formulation

For the admissible displacements $\boldsymbol{u}$ and the internal states z we choose the natural function spaces

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

Later we will also need the larger space $\mathscr{X} \stackrel{\text{def}}{=} \mathrm{L}^2(\Omega, \mathbb{R}^d \times \mathbb{R}^{d\times d}_{\mathrm{dev}})$. The symbol $\langle \cdot, \cdot \rangle$ denotes the duality pairing between $\mathscr{Q}'$ and $\mathscr{Q}$. For the loadings $\boldsymbol{f}$ and $\boldsymbol{T}$ in (3d) we require that $\boldsymbol{\ell}$ defined via

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

satisfies $\boldsymbol{\ell} \in \mathbf{C}^1([0,T]; \mathscr{X}')$. Furthermore, we choose an initial datum $q_0 = (\boldsymbol{u}_0, z_0) \in \mathscr{S}(0)$ where the set $\mathscr{S}(t)$ of *stable states at time* $t \in [0,T]$ is defined as the set of all $q = (\boldsymbol{u}, z) \in \mathscr{Q}$ satisfying the condition

$$\int_\Omega W(\boldsymbol{u}, z) \, \mathrm{d}x - \langle \boldsymbol{\ell}(t), q \rangle \leq \int_\Omega W(\boldsymbol{u}, z) \, \mathrm{d}x - \langle \boldsymbol{\ell}(t), q \rangle + \int_\Omega R|\widehat{z} - z| \, \mathrm{d}x \tag{4}$$

for all $\widehat{q} = (\widehat{\boldsymbol{u}}, \widehat{z}) \in \mathscr{Q}$.

The variational formulation of (3) consists in finding $q : [0,T] \to \mathscr{Q}$ such that

$$
\begin{aligned}
& q(0) = q_0, && \text{(5a)}\\
& \int_\Omega \mathbf{C}(\varepsilon(\boldsymbol{u}) - z) : \varepsilon(\boldsymbol{v})\,\mathrm{d}x = \langle \boldsymbol{\ell}, \boldsymbol{v}\rangle \quad \text{for all } \boldsymbol{v} \in \mathscr{U}, && \text{(5b)}\\
& \int_\Omega \big((\mathbf{C}(z - \varepsilon(\boldsymbol{u})) + \mathrm{D}_z H(z)) : (w - \dot z) + \nu \nabla z : \nabla(w - \dot z)\big)\,\mathrm{d}x \\
& \qquad + \int_\Omega R|w|\,\mathrm{d}x - \int_\Omega R|\dot z|\,\mathrm{d}x \geq 0 \quad \text{for all } w \in \mathscr{Z}, && \text{(5c)}
\end{aligned}
$$

almost everywhere in time. The following wellposedness theorem is proved in [AMS08], see also [Mie06, Sec. 5.3].

Theorem 1 (Wellposedness). *For each* $q_0 \in \mathscr{S}(0)$ *problem* (5) *admits a unique solution* $q : [0,T] \to \mathscr{Q}$*, which even lies in* $\mathbf{C}^{\mathrm{Lip}}([0,T];\mathscr{Q})$.

4 Space-time discretization: main result

Let us now introduce our space-time discretization of (5). To this aim, we choose a sequence $(\Pi_\tau)_{\tau>0}$ of partitions $\{\, 0 = t_\tau^0 < t_\tau^1 < \cdots < t_\tau^{k_\tau} = T \,\}$ of the time interval $[0,T]$ with $\max\{ t_\tau^k - t_\tau^{k-1} \,:\, k = 1,...,k_\tau\} \leq \tau$ and a sequence $(\mathscr{Q}_h)_{h>0}$ of finite-dimensional spaces exhausting $\mathscr{Q}$. In particular, assume to be given a regular triangulation $\{\mathscr{T}_k\}$ of Ω [QuV94] and choose $\mathscr{U}_h$ and $\mathscr{Z}_h$ to be the subspaces of continuous, piecewise polynomials of fixed degree $m \geq 1$ on $\{\mathscr{T}_k\}$. Finally, let $\mathscr{Q}_h \stackrel{\text{def}}{=} \mathscr{U}_h \times \mathscr{Z}_h$. As for the initial value, we shall ask for $q_{0,h} \in \mathscr{S}_h(0)$ where the set of *approximate stable states* is defined as in (4) by replacing $\mathscr{Q}$ by $\mathscr{Q}_h$.

Our space-time discretization of (5) consists in finding $q_{\tau,h}^i = (\boldsymbol{u}_{\tau,h}^i, z_{\tau,h}^i) \in \mathscr{Q}_h$ for $i = 0,1,\ldots,k_\tau$ such that

$$
\begin{aligned}
& q_{\tau,h}^0 = q_{0,h}, && \text{(6a)}\\
& \int_\Omega \mathbf{C}(\varepsilon(\boldsymbol{u}_{\tau,h}^i) - z_{\tau,h}^i) : \varepsilon(\boldsymbol{v}_h)\,\mathrm{d}x = \langle \boldsymbol{\ell}(t_\tau^i), \boldsymbol{v}_h\rangle \quad \text{for all } \boldsymbol{v}_h \in \mathscr{U}_h, && \text{(6b)}\\
& \int_\Omega \big(\mathbf{C}(z_{\tau,h}^i - \varepsilon(\boldsymbol{u}_{\tau,h}^i)) + \mathrm{D}_z H(z_{\tau,h}^i) : (w_h - \delta z_{\tau,h}^i) + \nu \nabla z_{\tau,h}^i : \nabla(w_h - \delta z_{\tau,h}^i)\big)\,\mathrm{d}x \\
& \qquad + \int_\Omega R|w_h|\,\mathrm{d}x - \int_\Omega R|\delta z_{\tau,h}^i|\,\mathrm{d}x \geq 0 \quad \text{for all } w_h \in \mathscr{Z}_h && \text{(6c)}
\end{aligned}
$$

for $i = 1,\ldots,k_\tau$. Here we used the short-hand notation

$$
\delta z_{\tau,h}^i \stackrel{\text{def}}{=} \frac{1}{t_\tau^i - t_\tau^{i-1}}\,(z_{\tau,h}^i - z_{\tau,h}^{i-1}),
$$

which will also be used for $q_{\tau,h}^i$ later on. Because of convexity the conditions (6b)-(6c) are equivalent to solving incremental minimization problems, see [Mie05].

We shall denote by $q_{\tau,h} = (\boldsymbol{u}_{\tau,h}, z_{\tau,h}) : [0,T] \to \mathscr{Q}_h \subset \mathscr{Q}$ the piecewise-constant-in-time interpolants of the above fully-discrete solutions. In particular,

$$q_{\tau,h}(t) \stackrel{\text{def}}{=} q_{\tau,h}^{k-1} \quad \text{for } t_\tau^{k-1} \le t < t_\tau^k,\ k = 1,\dots,k_\tau \quad \text{and} \quad q_{\tau,h}(T) \stackrel{\text{def}}{=} q_{\tau,h}^{k_\tau}.$$

The above scheme has been proved to be wellposed and convergent in [AMS08] (but see also [MiT04] and the detailed analysis of [MP*08, Appendix]).

Theorem 2 (Wellposedness, stability, and convergence). *For all $q_{0,h} \in \mathscr{S}_h(0)$, there exists a unique $q_{\tau,h}^i$ solving* (6)*. Moreover, there exists $C_{\text{stab}} > 0$ such that*

$$\|q_{\tau,h}^i\|_{\mathscr{Q}} + \big\|\delta q_{\tau,h}^i\big\|_{\mathscr{Q}} \le C_{\text{stab}} \quad \textit{for all } i = 1,\dots,k_\tau \textit{ and all } h > 0.$$

If additionally $q_{0,h} \to q_0$ in $\mathscr{Q}$, then $\max_{t\in[0,T]} \|q_{\tau,h}(t) - q(t)\|_{\mathscr{Q}}$ converges to 0 as $\tau + h \to 0$, where $q : [0,T] \to \mathscr{Q}$ is the unique solution of Theorem 1.

The purpose of this work is to establish a quantitative convergence result giving explicit convergence rates with respect to the mesh size h of the spatial discretization and the timestep τ. Our main result reads as follows:

Theorem 3 (Space-time convergence rates). *There exist $\alpha \in (0,1]$ and $C_{\text{err}} > 0$ (all independent from τ and h) such that the following holds. For each $q_0 \in \mathscr{S}(0)$ there exists a sequence $q_{0,h} \in \mathscr{S}_h(0)$ of approximating initial data, such that*

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

where q and $q_{\tau,h}$ are the unique solutions of (5) *and* (6)*, respectively. In case Ω is convex and $\Gamma_{\text{Neu}} = \emptyset$, one can choose $\alpha = 1$.*

A proof of this error estimate has been obtained in [MP*08] in the more general setting of an abstract evolutionary inequality. In the present concrete situation of SMAs the error-control argument is somehow simpler. Hence we are able to provide a full proof below.

5 Proof of the error estimate

Define the functionals $\mathscr{E} : [0,T] \times \mathscr{Q} \to \mathbb{R}$, $\mathscr{H} : \mathscr{Q} \to \mathbb{R}$, and $\Psi : \mathscr{Q} \to [0,\infty]$ via

$$\mathscr{E}(t,q) \stackrel{\text{def}}{=} \int_\Omega W(\boldsymbol{u},z)\,\mathrm{d}x - \langle \boldsymbol{\ell}(t), q\rangle\,,$$
$$\mathscr{H}(q) \stackrel{\text{def}}{=} \int_\Omega \Big(H(z) - \frac{c_2}{2}|z|^2\Big)\,\mathrm{d}x, \qquad \Psi(q) \stackrel{\text{def}}{=} \int_\Omega R|z|\,\mathrm{d}x.$$

In particular, note that there exists $C_\Psi > 0$ such that, for all $q \in \mathscr{Q}$, we have that $\Psi(q) \le C_\Psi \|q\|_{\mathscr{X}}$. Let $\mathbf{A} \in \text{Lin}(\mathscr{Q}, \mathscr{Q}')$ be defined by

$$\mathbf{A}q \stackrel{\text{def}}{=} \mathrm{D}_q\mathscr{E}(t,q) - \mathrm{D}_q\mathscr{H}(q) + \boldsymbol{\ell}(t),$$

that is, for all $(\boldsymbol{v},w) \in \mathscr{Q}$,

$$\langle \mathbf{A}(\boldsymbol{u},z),(\boldsymbol{v},w)\rangle \stackrel{\text{def}}{=} \int_\Omega \Big(\mathbf{C}(\varepsilon(\boldsymbol{u})-z):(\varepsilon(\boldsymbol{v})-w) + c_2 z{:}w + \nu\nabla z{:}\nabla w\Big)\,\mathrm{d}x.$$

Note that $\mathbf{A}$ is symmetric and coercive, namely there exists $\kappa > 0$ such that $\langle \mathbf{A}q,q\rangle \geq \kappa\|q\|^2_{\mathscr{Q}}$ for all $q \in \mathscr{Q}$. Finally, let $\mathbf{P}_h : \mathscr{Q} \to \mathscr{Q}_h$ be the Galerkin projector via $\mathbf{A}$, which is defined such that $\mathbf{P}_h q$ is the unique solution of

$$\langle \mathbf{A}\mathbf{P}_h q, p_h\rangle = \langle \mathbf{A}q, p_h\rangle \quad \text{for all } p_h \in \mathscr{Q}_h. \tag{7}$$

The Galerkin projectors $\mathbf{P}_h$ are uniformly bounded with respect to h and commute with $\mathbf{A}$, i.e., $\mathbf{P}_h^*\mathbf{A} = \mathbf{A}\mathbf{P}_h$.

The next lemma provides a useful approximation property of the Galerkin projectors. Note that this lemma crucially relies on the H^{1+s}-regularity of the associated linearized stationary problem for (5). Let $\mathbf{I}$ be the identity on $\mathscr{Q}$.

Lemma 1 (Approximation property). *There exist $\alpha \in (0,1]$ and $C_{\mathbf{P}} > 0$ such that*

$$\|(\mathbf{P}_h - \mathbf{I})q\|_{\mathscr{X}} \leq C_{\mathbf{P}} h^\alpha \|q\|_{\mathscr{Q}} \quad \textit{for all } h > 0 \textit{ and all } q \in \mathscr{Q}. \tag{8}$$

If Ω is convex and $\Gamma_{\mathrm{Neu}} = \emptyset$ then α can be chosen as $\alpha = 1$.

Proof. Within this proof, the symbol C stands for a generic positive constant, possibly depending on data only. Let us start by recalling that, in the present setting, given $\boldsymbol{f} \in \mathrm{L}^2(\Omega;\mathbb{R}^d)$, the unique solution $\boldsymbol{u} \in \mathscr{U}$ of the boundary value problem of linearized elastostatics

$$\int_\Omega \mathbf{C}\varepsilon(\boldsymbol{v}){:}\varepsilon(\boldsymbol{u})\,\mathrm{d}x = \int_\Omega \boldsymbol{f}\cdot\boldsymbol{v}\,\mathrm{d}x \quad \text{for all } \boldsymbol{v} \in \mathscr{U}$$

belongs to $\mathrm{H}^{1+s}(\Omega;\mathbb{R}^d)$ for some $s \in (0,1]$ and $s = 1$ for Ω convex and $\Gamma_{\mathrm{Neu}} = \emptyset$ [Gri92, Section 4.6, p. 148]. At the same time, given $g \in \mathrm{L}^2(\Omega;\mathbb{R}^{d\times d}_{\mathrm{dev}})$, the unique solution $z \in \mathscr{Z}$ of the elliptic system

$$\int_\Omega \Big(\mathbf{C}w{:}z + \nu\nabla w{:}\nabla z + c_2 w{:}z\Big)\,\mathrm{d}x = \int_\Omega g{:}w\,\mathrm{d}x \quad \text{for all } w \in \mathscr{Z}$$

is such that $z \in \mathrm{H}^{1+r}(\Omega;\mathbb{R}^{d\times d}_{\mathrm{dev}})$ for some $r \in (0,1]$ with $r = 1$ if Ω is convex [Gri92, Corollary 2.6.7, p. 79].

Let now $\eta = (\boldsymbol{f},g) \in \mathscr{X}'$ be given and $\varphi = (\boldsymbol{u},z) \in \mathscr{Q}$ be the unique solution of $\mathbf{A}^*\varphi = \eta$. By the very definition of $\mathbf{A}$ we get that

$$\int_\Omega \mathbf{C}\varepsilon(\boldsymbol{v}){:}\varepsilon(\boldsymbol{u})\,\mathrm{d}x = \int_\Omega (\boldsymbol{f} - \mathrm{div}(\mathbf{C}z))\cdot\boldsymbol{v}\,\mathrm{d}x \quad \text{for all } v \in \mathscr{U},$$
$$\int_\Omega (\mathbf{C}w{:}z + \nu\nabla w{:}\nabla z + c_2 w{:}z)\,\mathrm{d}x = \int_\Omega (g + \mathbf{C}\varepsilon(\boldsymbol{u})){:}w\,\mathrm{d}x \quad \text{for all } w \in \mathscr{Z}.$$

Owing to the above-recalled regularity theory we have that $\alpha \stackrel{\text{def}}{=} \min\{s,r\} \in (0,1]$ is such that

$$\|\varphi\|_{\mathrm{H}^{1+\alpha}(\Omega;\mathbb{R}^d\times\mathbb{R}^{d\times d}_{\mathrm{dev}})} \leq C\|(\boldsymbol{f}-\mathrm{div}(\mathbf{C}z), g+\mathbf{C}\varepsilon(\boldsymbol{u}))\|_{\mathscr{X}'} \leq C(\|\eta\|_{\mathscr{X}'}+\|\varphi\|_{\mathscr{Q}})$$

where $\alpha = 1$ for Ω convex and $\Gamma_{\mathrm{Neu}} = \emptyset$. In particular, as clearly $\|\varphi\|_{\mathscr{Q}} \leq C\|\eta\|_{\mathscr{X}'}$, we have proved the regularity

$$\|\varphi\|_{\mathrm{H}^{1+\alpha}(\Omega;\mathbb{R}^d\times\mathbb{R}^{d\times d}_{\mathrm{dev}})} \leq C\|\eta\|_{\mathscr{X}'}. \tag{9}$$

Next, we exploit the classical duality technique by Aubin and Nitsche [Aub67, Nit68]. Assume to be given a (linear) projector $\boldsymbol{\Pi}_h : \mathscr{Q} \to \mathscr{Q}_h$ fulfilling

$$\begin{aligned} &\text{for all } \sigma \in (0,1]\ \exists C > 0 \text{ for all } \widehat{\varphi} \in \mathscr{Q}\ : \\ &\|\widehat{\varphi}-\boldsymbol{\Pi}_h\widehat{\varphi}\|_{\mathscr{Q}} \leq Ch^{\sigma}\|\widehat{\varphi}\|_{\mathrm{H}^{1+\sigma}(\Omega;\mathbb{R}^d\times\mathbb{R}^{d\times d}_{\mathrm{dev}})}. \end{aligned} \tag{10}$$

The latter can be realized, for instance, by taking L^2-projections and the interpolation error control of (10) follows from [HP*05, Lemma 5.6]. Let $q \in \mathscr{Q}$ be fixed and define $\varphi \in \mathscr{Q}$ as the unique solution of $\mathbf{A}^*\varphi = (\mathbf{P}_h-\mathbf{I})q \in \mathscr{X}'$. We have that, for all $\varphi_h \in \mathscr{Q}_h$,

$$\begin{aligned} &\|(\mathbf{P}_h-\mathbf{I})q\|^2_{\mathscr{X}} = \langle \mathbf{A}^*\varphi, (\mathbf{P}_h-\mathbf{I})q\rangle = \langle \mathbf{A}(\mathbf{P}_h-\mathbf{I})q, \varphi\rangle \stackrel{(7)}{=} \langle \mathbf{A}(\mathbf{P}_h-\mathbf{I})q, \varphi-\varphi_h\rangle \\ &\leq \|\mathbf{A}\|_{\mathrm{Lin}(\mathscr{Q},\mathscr{Q}')}\|(\mathbf{P}_h-\mathbf{I})q\|_{\mathscr{Q}}\|\varphi-\varphi_h\|_{\mathscr{Q}} \leq C\|q\|_{\mathscr{Q}}\|\varphi-\varphi_h\|_{\mathscr{Q}}. \end{aligned}$$

By choosing $\varphi_h \stackrel{\text{def}}{=} \boldsymbol{\Pi}_h\varphi$ we get that

$$\begin{aligned} &\|(\mathbf{P}_h-\mathbf{I})q\|^2_{\mathscr{X}} \leq C\|q\|_{\mathscr{Q}}\|\varphi-\boldsymbol{\Pi}_h\varphi\|_{\mathscr{Q}} \\ &\stackrel{(10)}{\leq} C\|q\|_{\mathscr{Q}}h^{\alpha}\|\varphi\|_{\mathrm{H}^{1+\alpha}(\Omega;\mathbb{R}^d\times\mathbb{R}^{d\times d}_{\mathrm{dev}})} \stackrel{(9)}{\leq} C\|q\|_{\mathscr{Q}}h^{\alpha}\|(\mathbf{P}_h-\mathbf{I})q\|_{\mathscr{X}} \end{aligned}$$

and the assertion follows.

The core of the proof of Theorem 3 is contained in the following proposition.

Proposition 1 (Key estimate). *There exist $\alpha \in (0,1]$ and $C_{\mathrm{key}} > 0$ independent of τ and h such that*

$$\max_{t\in[0,T]} \|q(t)-q_{\tau,h}(t)\|_{\mathscr{Q}} \leq C_{\mathrm{key}}\big(\|q_0-q_{0,h}\|_{\mathscr{Q}}+h^{\alpha/2}+\tau^{1/2}\big).$$

Moreover, if Ω is convex and $\Gamma_{\mathrm{Neu}} = \emptyset$ then α can be chosen as $\alpha = 1$.

Proof. We clearly have that, for all $t \in [0,T]$,

$$\|q_{\tau,h}(t)-q(t)\|_{\mathscr{Q}} \leq \|q_{\tau,h}(t)-q_h(t)\|_{\mathscr{Q}} + \|q_h(t)-q(t)\|_{\mathscr{Q}}. \tag{11}$$

The first term in the above right-hand side can be estimated by using the same ideas of [MiT04, Prop. 7.2, Theorem 7.3]. Namely, there exists $C_1 > 0$ such that

$$\|q_{\tau,h}(t)-q_h(t)\|_{\mathscr{Q}} \leq C_1\tau^{1/2}. \tag{12}$$

We estimate now the second term on the right hand side of (11). Since q and q_h solve $(\mathscr{Q},\mathscr{E},\boldsymbol{\Psi},q_0)$ and $(\mathscr{Q}_h,\mathscr{E},\boldsymbol{\Psi},q_{0,h})$, respectively, we have

$$\langle \mathrm{D}_q\mathscr{E}(t,q_h(t)),v_h-\dot{q}_h(t)\rangle + \boldsymbol{\Psi}(v_h) - \boldsymbol{\Psi}(\dot{q}_h(t)) \geq 0 \quad \text{ for all } v_h \in \mathscr{Q}_h, \tag{13}$$
$$\langle \mathrm{D}_q\mathscr{E}(t,q(t)),v-\dot{q}(t)\rangle + \boldsymbol{\Psi}(v) - \boldsymbol{\Psi}(\dot{q}(t)) \geq 0 \quad \text{ for all } v \in \mathscr{Q}, \tag{14}$$

which hold a.e. in $[0,T]$. Choosing $v=\dot{q}_h(t)$ in (14) and adding it to (13) we obtain

$$\langle \mathrm{D}_q\mathscr{E}(t,q_h(t)),v_h-\dot{q}_h(t)\rangle + \langle \mathrm{D}_q\mathscr{E}(t,q(t)),\dot{q}_h(t)-\dot{q}(t)\rangle + \boldsymbol{\Psi}(v_h) - \boldsymbol{\Psi}(\dot{q}(t)) \geq 0,$$

for all $v_h \in \mathscr{Q}_h$. Using the triangle inequality this implies

$$\begin{aligned}&\langle \mathrm{D}_q\mathscr{E}(t,q_h(t))-\mathrm{D}_q\mathscr{E}(t,q(t)),\dot{q}_h(t)-\dot{q}(t)\rangle \\ &\quad \leq \langle \mathrm{D}_q\mathscr{E}(t,q_h(t)),v_h-\dot{q}(t)\rangle + \boldsymbol{\Psi}(v_h-\dot{q}(t)) \quad \text{ for all } v_h \in \mathscr{Q}_h.\end{aligned} \tag{15}$$

Let us now evaluate the right-hand side of (15) by computing, for all $v_h \in \mathscr{Q}_h$,

$$\begin{aligned}&\langle \mathrm{D}_q\mathscr{E}(t,q_h(t)),v_h-\dot{q}(t)\rangle + \boldsymbol{\Psi}(v_h-\dot{q}(t)) \\ &\leq \langle \mathbf{A}q_h(t),v_h-\dot{q}(t)\rangle + \big(\|\mathrm{D}_q\mathscr{H}(q_h(t))\|_{\mathscr{X}'} + \|\boldsymbol{\ell}(t)\|_{\mathscr{X}'} + C_{\Psi}\big)\|v_h-\dot{q}(t)\|_{\mathscr{X}}.\end{aligned}$$

Using $\mathrm{D}_q\mathscr{H} \in \mathbf{C}^{\mathrm{Lip}}(\mathscr{Q},\mathscr{X}')$ and letting $v_h = \mathbf{P}_h\dot{q}(t)$, we find $C_2>0$ such that

$$\begin{aligned}&\langle \mathbf{A}q_h(t)+\mathrm{D}_q\mathscr{H}(q_h(t))-\boldsymbol{\ell}(t),v_h-\dot{q}(t)\rangle + \boldsymbol{\Psi}(v_h-\dot{q}(t)) \\ &\leq \langle \mathbf{A}q_h(t),(\mathbf{P}_h-\mathbf{I})\dot{q}(t)\rangle + C_2\big(1+\|q_h(t)\|_{\mathscr{Q}}+\|q(t)\|_{\mathscr{Q}}\big)\|(\mathbf{P}_h-\mathbf{I})\dot{q}(t)\|_{\mathscr{X}}.\end{aligned}$$

Theorems 1 and 2 give $\|q_h(t)\|_{\mathscr{Q}} \leq C_{\mathrm{stab}}$, $\|q(t)\|_{\mathscr{Q}} \leq C_{\mathrm{stab}}$ and $\|\dot{q}(t)\|_{\mathscr{Q}} \leq C_{\mathrm{Lip}}$. Hence, using (7)-(8) and setting $C_3 \overset{\mathrm{def}}{=} \big(0+C_2C_{\mathbf{P}}(1+2C_{\mathrm{stab}})\big)C_{\mathrm{Lip}}$ we infer from (15) that

$$\langle \mathrm{D}_q\mathscr{E}(t,q_h(t))-\mathrm{D}_q\mathscr{E}(t,q(t)),\dot{q}_h(t)-\dot{q}(t)\rangle \leq C_3h^{\alpha}\|\dot{q}(t)\|_{\mathscr{Q}}. \tag{16}$$

Define $\gamma(t) \overset{\mathrm{def}}{=} \langle \mathrm{D}_q\mathscr{E}(t,q_h(t))-\mathrm{D}_q\mathscr{E}(t,q(t)),q_h(t)-q(t)\rangle \geq \kappa\|q_h(t)-q(t)\|^2_{\mathscr{Q}}$ where the lower bound stems from the coercivity of $\mathbf{A}$ and the convexity of $\mathscr{H}$. We have

$$\begin{aligned}\dot{\gamma}(t) &= 2\langle \mathrm{D}_q\mathscr{E}(t,q_h)-\mathrm{D}_q\mathscr{E}(t,q),\dot{q}_h-\dot{q}\rangle + \langle \partial_t\mathrm{D}_q\mathscr{E}(t,q_h)-\partial_t\mathrm{D}_q\mathscr{E}(t,q),q_h-q\rangle \\ &\quad + \langle \mathrm{D}_q\mathscr{E}(t,q)-\mathrm{D}_q\mathscr{E}(t,q_h)+\mathrm{D}_q^2\mathscr{E}(t,q_h)[q_h-q],\dot{q}_h\rangle \\ &\quad + \langle \mathrm{D}_q\mathscr{E}(t,q_h)-\mathrm{D}_q\mathscr{E}(t,q)+\mathrm{D}_q^2\mathscr{E}(t,q)[q-q_h],\dot{q}\rangle.\end{aligned}$$

Exploiting $\mathrm{D}_q\mathscr{H} \in \mathbf{C}^{1,\mathrm{Lip}}(\mathscr{Q},\mathscr{Q}')$ and estimate (16) provides $C_4>0$ such that

$$\dot{\gamma} \leq 2C_3h^{\alpha}\|\dot{q}\|_{\mathscr{Q}} + C_4\big(0+\|\dot{q}\|_{\mathscr{Q}}+\|\dot{q}_h\|_{\mathscr{Q}}\big)\|q_h-q\|^2_{\mathscr{Q}}. \tag{17}$$

Setting $C_5 \overset{\mathrm{def}}{=} \max(2C_3,C_4(0+2C_{\mathrm{Lip}}))$, we deduce from the definition of γ and (17) that we have $\dot{\gamma}(t) \leq C_5\big(h^{\alpha}+\gamma(t)/\kappa\big)$. Hence Gronwall's lemma yields $\gamma(t) \leq$

$\big(\mathrm{e}^{C_5 t/\kappa}-1\big)\kappa h^\alpha+\mathrm{e}^{C_5 t/\kappa}\gamma(0)$. As we readily infer that $\gamma(0)\leq C_6\|q_{0,h}-q_0\|^2_{\mathscr{Q}}/\kappa$ with $C_6 \stackrel{\mathrm{def}}{=} \|\mathbf{A}\|_{\mathrm{Lin}(\mathscr{Q},\mathscr{Q}')}+C_{\mathscr{H}}$ for $C_{\mathscr{H}} \stackrel{\mathrm{def}}{=} \|\mathrm{D}_q\mathscr{H}\|_{\mathrm{Lip}}$, we have obtained that

$$\|q_h(t)-q(t)\|^2_{\mathscr{Q}} \leq \big(\mathrm{e}^{C_5 t/\kappa}-1\big)h^\alpha + C_6\mathrm{e}^{C_5 t/\kappa}\|q_{0,h}-q_0\|^2_{\mathscr{Q}}/\kappa. \tag{18}$$

Carrying (12) and (18) into (11) we obtain the desired result.

Once Proposition 1 is established, the proof of Theorem 3 is concluded by the following approximation result for initial data.

Lemma 2 (Approximation of initial data). *There exists $C_0>0$ and a choice of approximated initial conditions $q_{0,h}\in\mathscr{S}_h(0)$ such that, for h small,*

$$\|q_0-q_{0,h}\|_{\mathscr{Q}} \leq C_0 h^{\alpha/2} \ \textit{where}\ \alpha\in(0,1]\ \textit{is the same as in}\ (8).$$

Proof. The approximations $q_{0,h}$ may be obtained by solving the following problem $q_{0,h}=\mathrm{Argmin}_{\widehat{q}_h\in\mathscr{Q}_h}\{\mathscr{E}(0,\widehat{q}_h)+\Psi(\widehat{q}_h-\mathbf{P}_hq_0)\}$. By the triangle inequality, we find

$$\begin{aligned}\mathscr{E}(0,q_{0,h}) &\leq \mathscr{E}(0,\widehat{q}_h)+\Psi(\widehat{q}_h-\mathbf{P}_hq_0)-\Psi(q_{0,h}-\mathbf{P}_hq_0)\\ &\leq \mathscr{E}(0,\widehat{q}_h)+\Psi(\widehat{q}_h-q_{0,h}),\end{aligned} \tag{19}$$

for all $\widehat{q}_h\in\mathscr{Q}_h$. Namely, we have proved that $q_{0,h}\in\mathscr{S}_h(0)$. Since $q_0\in\mathscr{S}(0)$, we have $\mathscr{E}(0,q_0)+\frac{\kappa}{2}\|\widehat{q}-q_0\|^2_{\mathscr{Q}}\leq\mathscr{E}(0,\widehat{q})+\Psi(\widehat{q}-q_0)$ for all $\widehat{q}\in\mathscr{Q}$. Letting $\widehat{q}=q_{0,h}$ and using the triangle inequality and the minimality of $q_{0,h}$ we obtain

$$\begin{aligned}\frac{\kappa}{2}\|q_{0,h}-q_0\|^2_{\mathscr{Q}} &\leq \mathscr{E}(0,q_{0,h})-\mathscr{E}(0,q_0)+\Psi(q_{0,h}-\mathbf{P}_hq_0)+\Psi((\mathbf{P}_h-\mathbf{I})q_0)\\ &\stackrel{(19)}{\leq} \mathscr{E}(0,\widehat{q}_h)-\mathscr{E}(0,q_0)+\Psi(\widehat{q}_h-\mathbf{P}_hq_0)+\Psi((\mathbf{P}_h-\mathbf{I})q_0)\end{aligned}$$

for all $\widehat{q}_h\in\mathscr{Q}_h$. When choosing $\widehat{q}_h=\mathbf{P}_hq_0$ we find

$$\frac{\kappa}{2}\|q_{0,h}-q_0\|^2_{\mathscr{Q}} \leq \mathscr{E}(0,\mathbf{P}_hq_0)-\mathscr{E}(0,q_0)+\Psi((\mathbf{P}_h-\mathbf{I})q_0). \tag{20}$$

Next, we evaluate the right hand side of (20) as follows

$$\begin{aligned}&\frac{\kappa}{2}\|q_{0,h}-q_0\|^2_{\mathscr{Q}} \leq \mathscr{E}(0,\mathbf{P}_hq_0)-\mathscr{E}(0,q_0)+\Psi((\mathbf{P}_h-\mathbf{I})q_0)\\ &=\langle\mathbf{A}\mathbf{P}_hq_0,(\mathbf{P}_h-\mathbf{I})q_0\rangle-\frac{1}{2}\langle\mathbf{A}(\mathbf{P}_h-\mathbf{I})q_0,(\mathbf{P}_h-\mathbf{I})q_0\rangle\\ &\qquad+\mathscr{H}(\mathbf{P}_hq_0)-\mathscr{H}(q_0)-\langle\boldsymbol{\ell}(0),(\mathbf{P}_h-\mathbf{I})q_0\rangle+\Psi((\mathbf{P}_h-\mathbf{I})q_0)\\ &\stackrel{(7)}{=}-\frac{1}{2}\langle\mathbf{A}(\mathbf{P}_h-\mathbf{I})q_0,(\mathbf{P}_h-\mathbf{I})q_0\rangle-\langle\boldsymbol{\ell}(0),(\mathbf{P}_h-\mathbf{I})q_0\rangle+\Psi((\mathbf{P}_h-\mathbf{I})q_0)\\ &\qquad+\int_0^1\langle\mathrm{D}_q\mathscr{H}(q_0+s(\mathbf{P}_h-\mathbf{I})q_0),(\mathbf{P}_h-\mathbf{I})q_0\rangle\,\mathrm{d}s.\end{aligned} \tag{21}$$

The integral term in the above right-hand side can be estimated as follows

$$\begin{aligned}
&\int_0^1 \langle \mathrm{D}_q \mathscr{H}(q_0+s(\mathbf{P}_h-\mathbf{I})q_0), (\mathbf{P}_h-\mathbf{I})q_0\rangle \,\mathrm{d}s \\
&= \int_0^1 \langle \mathrm{D}_q \mathscr{H}(q_0+s(\mathbf{P}_h-\mathbf{I})q_0) - \mathrm{D}_q \mathscr{H}(q_0), (\mathbf{P}_h-\mathbf{I})q_0\rangle \,\mathrm{d}s \\
&+ \int_0^1 \langle \mathrm{D}_q \mathscr{H}(q_0), (\mathbf{P}_h-\mathbf{I})q_0\rangle \,\mathrm{d}s \\
&\le \int_0^1 s C_{\mathscr{H}} \|(\mathbf{P}_h-\mathbf{I})q_0\|_{\mathscr{Q}} \|(\mathbf{P}_h-\mathbf{I})q_0\|_{\mathscr{X}} \,\mathrm{d}s + \|\mathrm{D}_q \mathscr{H}(q_0)\|_{\mathscr{X}'} \|(\mathbf{P}_h-\mathbf{I})q_0\|_{\mathscr{X}}.
\end{aligned}$$

Hence, using (8) and (21), we find

$$\begin{aligned}
&\frac{\kappa}{2}\|q_{0,h}-q_0\|_{\mathscr{Q}}^2 + \frac{\kappa}{2}\|(\mathbf{P}_h-\mathbf{I})q_0\|_{\mathscr{Q}}^2 \\
&\overset{(21)}{\le} C_{\mathbf{P}} h^{\alpha} \|q_0\|_{\mathscr{Q}} \Big(\|\boldsymbol{\ell}(0)\|_{\mathscr{X}'} + C_{\Psi} + \frac{C_{\mathscr{H}}}{2} \|(\mathbf{P}_h-\mathbf{I})q_0\|_{\mathscr{Q}} + \|\mathrm{D}_q \mathscr{H}(q_0)\|_{\mathscr{X}'} \Big).
\end{aligned}$$

The assertion follows by taking h small.

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