Analysis of a variable time-step discretization for a phase transition model with micro-movements

Ulisse Stefanelli
Istituto di Matematica Applicata e Tecnologie Informatiche – CNR
via Ferrata 1, 27100 Pavia, Italy
e-mail: ulisse@imati.cnr.it

Abstract

This note deals with a semi-implicit time discretization with variable time-step of a phase transition model taking into account the microscopic movements of molecules. In particular, we focus on the study of an unconditionally stable and convergent approximation. Moreover, an *a priori* estimate for the discretization error is established.

Key words: phase transitions, microscopic movements, time discretization.

AMS (MOS) Subject Classification: 80A22, 35K55, 65M15.

1 Introduction

The present analysis is concerned with a nonlinear system of partial differential equations describing the evolution of the two unknown scalar fields θ and χ. Letting Ω be a bounded domain in $\mathbb{R}^n$ $(n = 1, 2, 3)$ and $T > 0$ be some final time, we deal with the following relations

$$\dot{\theta} + \theta\dot{\chi} - \Delta\theta = 0 \tag{1.1}$$

$$\dot{\chi} + \alpha(\dot{\chi}) - \Delta\chi + \beta(\chi) \ni \theta - \theta_c, \tag{1.2}$$

to be fulfilled almost everywhere in $\Omega \times (0, T)$. Here the dot stands for differentiation with respect to time, α denotes a maximal monotone graph in $\mathbb{R} \times \mathbb{R}$, β is a locally Lipschitz continuous monotone function, and θ_c is a given positive constant. In particular, we choose α to be the *subdifferential* of the indicator function of the set $[0, +\infty)$. Namely, we have

$$y \in \alpha(x) \ \text{ iff } \ x \geq 0 \ \text{ and } \ y(x - w) \geq 0 \ \ \forall w \geq 0, \tag{1.3}$$

or, equivalently, $\alpha(0) = (-\infty, 0]$, $\alpha(x) = 0$ for $x > 0$, and $\alpha(x) = \emptyset$ for $x < 0$.

The system (1.1)-(1.2) arises in connection with the description of solid-liquid phase transitions taking into account the microscopic movements of molecules. In the context of the mathematical modeling of phase transition phenomena it is indeed very common to regard the medium undergoing the phase transition as a *rigid body*. Although this assumption may be often fully justified at a macroscopic scale, it is clear that a phase transition is related to some change in the molecular arrangements in the medium. That is to say that the system that undergoes a phase change is surely not rigid at all at the microscopic level.

A new class of phase transition models taking into account *microscopic movements* of particles has been recently introduced by M. Frémond [12]. In the framework of this new theory, one still considers that the mechanical effect of the microscopic rearrangements of particles is *negligible* at the macro-scales, where it is assumed that the latter movements are somehow averaged out. Nevertheless, one admits that the microscopic movements of particles give actually rise to some thermal macroscopic effect which indeed influences the overall energy balance of the body. We shall mention that the idea of introducing a two-scale mechanical balance in order to describe some material effect is not new and has been for instance introduced within the framework of the Cahn-Hilliard equation by M.E. Gurtin [15] (see also [14] for additional details). In particular, in [15] a new balance law for the so-called *micro-forces* is coupled with the standard macroscopic balance equations. The above-mentioned theory, although it gives rise to differential models that turn out to be similar to those derived within Frémond's framework, has indeed an independent physical motivation. On the other hand let us mention that the mathematical problems related to the theory of micro-forces have recently attracted a substantial deal of interest [16, 24, 25, 26].

Let us now introduce a general model for solid-liquid phase transitions with microscopic movements. Assume we are given a regular domain $\Omega \subset \mathbb{R}^n$ $(n = 1, 2, 3)$, connected, with a smooth boundary $\Gamma := \partial\Omega$, and filled with a substance which may undergo a two-phase transformation. We aim to study the evolution of the system in a fixed time interval $[0, T]$ by means of the state variables θ (absolute temperature) and χ (order parameter). For the sake of convenience, let us introduce some notations for the cylinders $Q_t := \Omega \times (0, t)$, $\Sigma_t := \Gamma \times (0, t)$ for $t \in (0, T]$, and let $Q := Q_T$, $\Sigma := \Sigma_T$. Hence, by referring the reader to the original papers [4, 3] and the recent monograph [12] for a full justification from the point of view of Continuum Thermo-Mechanics, we are left with the study of the following system of relations

$$c_s\dot{\theta} + L\dot{\chi} - k\Delta\theta = -\frac{L}{\theta_c}(\theta - \theta_c)\dot{\chi} + \mu_1\dot{\chi}^2 + \xi\dot{\chi} + \delta|\nabla\dot{\chi}|^2, \tag{1.4}$$

$$\mu_2\dot{\chi} - \delta\Delta\dot{\chi} - \nu\Delta\chi + \xi + \eta = \frac{L}{\theta_c}(\theta - \theta_c), \tag{1.5}$$

$$\xi \in \gamma(\dot{\chi}), \quad \eta \in \beta(\chi). \tag{1.6}$$

Indeed, equation (1.4) represents the energy balance of the body while relations (1.5)-(1.6) stand for its micro-momentum balance. In the latter expressions c_s represents a specific heat density, L is a latent heat density, k is the constant thermal conductivity, and θ_c is the phase transition temperature. The physical parameters $\mu_1, \mu_2, \delta, \nu$ are non-negative and the reader is referred to [12] for their physical motivation. Moreover, β, γ are now maximal monotone graphs in $\mathbb{R} \times \mathbb{R}$. Let us stress from the very beginning that some physically interesting choices for γ are $\gamma = 0$ and $\gamma = \alpha$. We will refer to the first choice as the *reversible* situation while the second is termed *irreversible*. In particular, the choice $\gamma = \alpha$ is intended to force $\dot{\chi}$ to attain only non-negative values modeling indeed the situation of irreversible phase transitions [13] which includes, possibly, thermal hardening of glues, food cooking etc. Let us recall that, whenever $\gamma = \alpha$ or $\gamma = 0$ the term $\xi\dot{\chi}$ in the right hand side of (1.4) is 0 since $\xi \neq 0$ only if $\dot{\chi} = 0$. Moreover, we stress that in the original model one has $\mu_1 = \mu_2$ and that we specialized this notation for the sake of later purposes. As for β we have to remark that two physically interesting situations are that of a cubic nonlinearity arising from a double-well potential and the subdifferential ε of the indicator function of the interval $[0, 1]$ (especially suited for the case of χ being a phase proportion), namely

$$y \in \varepsilon(x) \;\text{ iff }\; x \in [0, 1] \;\text{ and }\; y(x - w) \geq 0 \;\; \forall w \in [0, 1],$$

or, equivalently, $\varepsilon(0) = (-\infty, 0]$, $\varepsilon(1) = [0, +\infty)$, $\varepsilon(x) = 0$ if $x \in (0, 1)$, and $\varepsilon(x) = \emptyset$ elsewhere. Since we are restricting ourselves to the case of a locally Lipschitz continuous function β we shall explicitly mention that the latter choice $\beta = \varepsilon$ is clearly not covered by the present analysis. On the other hand, we are entitled to consider the cubic nonlinearity case.

Instead of presenting a derivation of relations (1.4)-(1.6), we prefer to outline here a brief survey on the current literature on the model. The first result in the direction of the well-posedness for some model related to (1.4)-(1.6) can be found in [3]. In the latter paper the authors detail the derivation of the model in the case $\delta = 0$, and linearize (1.4) as

$$c_s\dot{\theta} + L\dot{\chi} - k\Delta\theta = 0, \tag{1.7}$$

obtaining indeed existence of strong solutions in the multidimensional setting for quite general graphs γ, β. Indeed, whenever the above linearized equation is coupled with (1.5)-(1.6) where $\nu = \delta = 0$, we have to quote the former contributions [1, 2] where the ODE structure of the momentum equation is fully investigated. Let us stress that the simplification assumption leading to (1.7) is twofold. From the one hand, one assumes to be interested in temperature regimes which are close to equilibrium ($\theta \simeq \theta_c$). From the other hand one neglects the second order term $\mu_1\dot{\chi}^2$ in the energy balance equation by assuming that indeed the phase transformation is very slow.

A first attempt in the direction of including the nonlinearities in (1.4) has been accomplished in [20] where the authors consider $\mu_1 = \delta = 0$ in the irreversible case $\gamma = \alpha$. Once again, the existence of a global strong solution is achieved in the multidimensional setting by means of a regularization technique. Of course here the model refers again to suitably slow phase changes, but one is allowed to consider situations far from the critical temperature θ_c. This is exactly the model problem that is reconsidered in this note from the point of view of its possible approximation.

The results of the paper [9] concern a system which is fully consistent from the modeling viewpoint, i.e. (1.4)-(1.6) with the choices $\beta = \varepsilon$ and $\delta = \nu = 0$. The analysis of [9] relies on the idea of carefully exploiting the ODE structure of (1.5) that occurs within this choice of parameters.

Again in the multidimensional setting, we have to quote [21] which focuses on the full model (1.4)-(1.6) with the choice $\delta = 0$. In the latter paper, the authors choose γ to be the indicator function of the interval $[0, \lambda]$ for some large $\lambda > 0$ representing a limiting velocity in the phase transition. The existence of a global strong solution is achieved by means of a time discretization argument, and it strongly relies on the a priori uniform bound on $\dot{\chi}$. Namely, $0 \leq \dot{\chi} \leq \lambda$.

The full three-dimensional problem (1.4)-(1.6) with $\delta = 0$, $\gamma = \alpha$, and $\beta = \varepsilon$ has been recently proved to admit a local in time strong solution by means of an approximation argument [30]. Let us stress that the locality (in time) of the above result is motivated by the highly nonlinear character of the problem. In particular, one has to use a generalized Gronwall-type lemma leading to local solvability [29, Thm. 7.1].

A different approach to this class of problems is addressed in [22] where the system (1.4)-(1.6) is suitably rewritten by means of some hysteresis relations. In particular, the authors investigate an extension of the results of [17] to the case when the energy balance equation is not assumed to be linear and takes the form of (1.4) with $\delta = 0$.

As for the one-dimensional case, we shall refer to the papers [18] and [23]. Here problem (1.4)-(1.6) is studied for $\delta = 0$ both in the reversible [23] and the irreversible situation [18]. The existence of a global strong solution is achieved by means of an approximation, a priori estimate, and passage to the limit technique inspired to some similar problems in thermo-visco-elasticity [10, 11]. In particular, some suitable estimates, available indeed just in the one-dimensional setting, are fully exploited. A further global solvability result is contained in [32] where the authors face the problem of finding a solution to the elliptic-parabolic problem (1.4)-(1.6) for $\mu_1 = \mu_2 = \delta = 0$ and either $\gamma = 0$ or $\gamma = \alpha$. The existence result is obtained by means of a suitable parabolic approximation ($\mu_2 > 0$) through a limit procedure.

We shall also mention the contributions [5, 6] where the effect of microscopic accelerations is taken into account and a well-posedness analysis for the related hyperbolic-parabolic problem is presented.

Finally, the strict positivity of the temperature has been proved in [31] for a very general class of models of the type of (1.4)-(1.6). In particular, this general result fully justifies the thermodynamic consistency of Frémond's approach for all the dissipative models of this class that have been considered in the literature.

This paper is devoted to the study of a variable time-step discretization procedure for the system (1.1)-(1.2). The latter system fits in the general frame of (1.4)-(1.6) with the choices $\mu_1 = \delta = 0$ and $\gamma = \alpha$ and the normalization of most of the constants to 1. The interest in implementing some numerical experiment is evident. Indeed, the possibility of devising some efficient approximation methods would both be crucial for applications and greatly serve for the sake of validating Frémond's approach. On the other hand, all of the models in (1.4)-(1.6) that have been proved so far to admit a solution are not known to be well-posed, in particular we are lacking uniqueness proofs. This fact, basically motivated by the highly nonlinear features of the models and often related also to the reduced and/or regularized problems, prevents somehow from obtaining an effective approximation procedure. In this paper we will focus on (1.1)-(1.2) which retains most of the basic issues of the modeling, admitting indeed a unique solution. We will study a suitable variable time-step discretization of the above problem, addressing unconditional stability and convergence issues. Finally, we will prove an a priori error bound on the discretization error.

Let us just stress that some time discretization techniques have already been exploited for the sake of proving existence results within the class of phase change models with micro movements [18, 21]. On the other hand, the original existence result of [20] is based on some regularization procedure and fixed point techniques. In particular, no discretization is proposed in [20]. In this concern, we provide here the basic ideas for an independent existence proof and some novel regularity result.

This is the plan of the paper. In Section 2 we will set some notation and state the problem in the continuous setting. The details on the variable time-step discretization are presented in Section 3 while its unconditional stability and convergence are proved in Section 4. Finally, Section 5 addresses the issue of error controlling.

2 Continuous problem

Let us start by defining

$$H := L^2(\Omega), \quad V := H^1(\Omega), \quad \text{and} \quad W := \{u \in H^2(\Omega) \ \text{ such that } \ \partial_\nu u = 0 \ \text{ on } \ \partial\Omega\},$$

endowed with the respective standard scalar products, where ν stands for the outward unit normal to $\partial\Omega$. In particular, we denote by $(\cdot,\cdot)$ and $\|\cdot\|$ the scalar product and the norm in H and by $\|\cdot\|_E$ the norm in the generic Banach space E. The reader is referred for instance to [19] for definitions and properties of function spaces.

We set the following assumptions on data. Let

$$0 \le \theta_c \le \theta_* \quad \text{be assigned constants,} \tag{2.1}$$

$$\alpha : \mathbb{R} \to 2^{\mathbb{R}} \quad \text{be defined by}$$

$$y \in \alpha(x) \ \text{ iff } \ x \ge 0 \ \text{ and } \ y(x-w) \ge 0 \ \ \forall w \ge 0, \tag{2.2}$$

$$j \in C^1(\mathbb{R}) \quad \text{be convex, } \min j = j(0) = 0,$$

$$\beta := j' \quad \text{be locally Lipschitz continuous,} \tag{2.3}$$

$$\theta_0 \in V \text{ and } \ 0 \le \theta_0 \le \theta_* \ \text{ a.e. in } \ \Omega, \tag{2.4}$$

$$\chi_0 \in W. \tag{2.5}$$

By collecting [20, Thm. 2.2] and [20, Prop. 2.4], we are able to state the following well-posedness result.

Theorem 2.1. *Let assumptions (2.1)-(2.5) hold. Then, there exists a unique triplet* (θ, χ, ξ) *such that*

$$\theta \in H^1(0,T;H) \cap C^0([0,T];V) \cap L^2(0,T;W), \tag{2.6}$$
$$\chi \in W^{1,\infty}(0,T;H) \cap H^1(0,T;V) \cap L^\infty(0,T;W), \tag{2.7}$$
$$\xi \in L^\infty(0,T;H), \tag{2.8}$$
$$\dot\theta + \theta\dot\chi - \Delta\theta = 0, \tag{2.9}$$
$$\dot\chi + \xi - \Delta\chi + \beta(\chi) = \theta - \theta_c \qquad a.e. \ in \ Q, \tag{2.10}$$
$$\xi \in \alpha(\dot\chi) \qquad a.e. \ in \ Q, \tag{2.11}$$
$$\theta(\cdot,0) = \theta_0, \quad \chi(\cdot,0) = \chi_0 \quad a.e. \ in \ \Omega. \tag{2.12}$$

Moreover, it turns out that

$$0 \le \theta \le \theta_* \qquad a.e. \ in \ Q. \tag{2.13}$$

Although we will not provide here explicitly a new proof of this result, let us just stress that the existence part is indeed a consequence of the forthcoming Lemma 4.2. As for uniqueness, we remark that indeed it may be proved by suitably reformulating (indeed in a rather simplified manner) the argument of Section 5.

Remark 2.2. Since for $n \le 3$ one has that W is embedded continuously into $L^\infty(\Omega)$, the regularity (2.7) entails that we may actually regard β as a globally Lipschitz continuous function without loss of generality.

Remark 2.3. The special choice of (2.2) could be generalized to

$$\alpha : \mathbb{R} \to 2^{\mathbb{R}} \quad \text{such that} \quad D(\alpha) \subset [0,+\infty) \quad \text{and} \quad 0 \in \alpha(0),$$

with no particular intricacy (here $D(\alpha) := \{x \in \mathbb{R} \ : \ \alpha(x) \neq \emptyset\}$ is the effective domain of α).

Before closing this section let us mention that we are actually in the position of sharpening the existence result of [20, Thm. 2.2] by requiring the extra regularity (see (2.5))

$$\eta_0 := (1+\alpha)^{-1}(\Delta\chi_0 - \beta(\chi_0) + \theta_0 - \theta_c) \in V, \tag{2.14}$$

where of course 1 stands for the identity in $\mathbb{R}$. Let us stress that (2.2)-(2.5) already entail that η_0 belongs to H. On the other hand, whenever $\chi_0 \in H^3(\Omega)$ we readily check that (2.14) holds. By suitably exploiting our discretization technique we will provide the following regularity result.

Lemma 2.4 (Regularity). *Let assumptions (2.1)-(2.14) hold. Then, the unique solution* (θ, χ, ξ) *to (2.6)-(2.12) fulfills*

$$\chi \in H^2(0,T;H) \cap W^{1,\infty}(0,T;V). \tag{2.15}$$

Of course, moving from (2.15), some extra regularity for θ will follow from standard parabolic estimates. Moreover, by restricting the choice in (2.4) to some more regular initial data we would be in the position of obtaining even sharper regularity results for θ. This will however drift our attention from our main focus on approximation issues and we prefer to leave it to the reader.

3 Discretization

Let us now focus on a possible approximation of the above system (2.9)-(2.12). We are interested in a *variable time-step discretization* of the problem. To this aim let us start by introducing the partition

$$\mathcal{P} := \{0 = t_0 < t_1 < \cdots < t_{N-1} < t_N = T\},$$

with variable time-step $\tau_i := t_i - t_{i-1}$ and let $\tau := \max_{1\le i\le N} \tau_i$ denote the diameter of the partition $\mathcal{P}$. No constraints are imposed on the possible choice of the time-steps throughout this analysis.

In the forthcoming discussion the following notation will be extensively used. Letting $\{u_i\}_{i=0}^N$ be a vector, we denote by $u_{\mathcal{P}}$ and $\overline{u}_{\mathcal{P}}$ two functions of the time interval $[0,T]$ which interpolate the values of the vector $\{u_i\}$ piecewise linearly and backward constantly on the partition $\mathcal{P}$, respectively. Namely

$$\begin{aligned} u_{\mathcal{P}}(0) &:= u_0, \quad u_{\mathcal{P}}(t) := \gamma_i(t)u_i + \big(1-\gamma_i(t)\big)u_{i-1}, \\ \overline{u}_{\mathcal{P}}(0) &:= u_0, \quad \overline{u}_{\mathcal{P}}(t) := u_i, \qquad \text{for } \ t \in (t_{i-1}, t_i], \quad i = 1,\ldots,N \end{aligned}$$

where

$$\gamma_i(t) := (t - t_{i-1})/\tau_i \quad \text{for } t \in (t_{i-1}, t_i], \quad i = 1,\ldots,N.$$

Moreover, we indicate with $\mathcal{T}_{\mathcal{P}}$ an operator acting on functions $\overline{u} : [0,T] \longrightarrow \mathbb{R}$ which are piecewise constant on $\mathcal{P}$ (i.e. $\overline{u}(t) = \overline{u}(t_i)$ for $t \in (t_{i-1}, t_i]$, $i = 1,\ldots,N$) and is defined by

$$(\mathcal{T}_{\mathcal{P}}\overline{u})(t) := \overline{u}(t_{i-1}) \quad \text{for } \ t \in (t_{i-1}, t_i], i = 1,\ldots,N.$$

Moreover, we will make use also of a quadratic interpolating function of $\{u_i\}_{i=-1}^N$. In particular, by assuming $\tau_0 > 0$ to be given and defining $\hat{u}'(0) := (u_0 - u_{-1})/\tau_0$, we let $\tilde{u} : [0,T] \longrightarrow \mathbb{R}$ be defined as

$$\tilde{u}_{\mathcal{P}}(t) := u_0 + \int_0^t \gamma_{\mathcal{P}}(s)u'_{\mathcal{P}}(s) + (1-\gamma_{\mathcal{P}}(s))\mathcal{T}_{\mathcal{P}}u'_{\mathcal{P}}(s)\, ds,$$

where $\gamma_{\mathcal{P}}(t) := \gamma_i(t)$ for $t \in (t_{i-1}, t_i]$, $i = 1,\ldots,N$. As for the latter interpolating function we shall stress that

$$\tilde{u}''_{\mathcal{P}}(t) = \frac{1}{\tau_i}\left(\frac{u_i - u_{i-1}}{\tau_i} - \frac{u_{i-1} - u_{i-2}}{\tau_{i-1}}\right) \quad \text{for } \ t \in (t_{i-1}, t_i], \ i = 1,\ldots,N. \tag{3.1}$$

The reader is referred to [33] for some additional material.

Let now $\theta_{0\mathcal{P}}, \chi_{0\mathcal{P}} \in W$ be some approximating initial data fulfilling (2.4). We are interested in finding a solution

$$\{\theta_i, \chi_i\}_{i=0}^N \in (W \times W)^{N+1}$$

to the scheme

$$\theta_0 = \theta_{0\mathcal{P}}, \quad \chi_0 = \chi_{0\mathcal{P}}, \tag{3.2}$$

$$\frac{\theta_i - \theta_{i-1}}{\tau_i} + \theta_i \frac{\chi_i - \chi_{i-1}}{\tau_i} - \Delta\theta_i = 0 \qquad i = 1,\ldots,N, \tag{3.3}$$

$$(1+\alpha)\left(\frac{\chi_i - \chi_{i-1}}{\tau_i}\right) - \Delta\chi_i + \beta(\chi_i) \ni \theta_{i-1} - \theta_c \qquad i = 1,\ldots,N. \tag{3.4}$$

In particular, we approximate time derivatives by means of the backward Euler method and we consider the right hand side of (3.4) to be known at each level i. This is to say that the above scheme is semi-implicit.

Our first result is the following well-posedness.

Lemma 3.1 (Discrete well-posedness). *The scheme (3.2)-(3.4) admits a unique solution.*

Proof. Let us proceed by induction on i. Namely, we shall prove that, given $(\theta_{i-1}, \chi_{i-1}) \in W \times W$, we may find $(\theta_i, \chi_i) \in W \times W$ fulfilling relations (3.3)-(3.4). As a first step we claim that one may find a unique $\chi_i \in W$ fulfilling (3.4). Unfortunately we cannot simply exploit the well-known results on the sum of maximal monotone nonlinearities in this particular setting and we are forced to introduce a further regularization parameter $\sigma > 0$ and study instead

$$(1+\alpha_\sigma)\left(\frac{\chi_{i,\sigma} - \chi_{i-1}}{\tau_i}\right) - \Delta\chi_{i,\sigma} + \beta(\chi_{i,\sigma}) = \theta_{i-1} - \theta_c \tag{3.5}$$

where α_σ is the standard Yosida approximation

$$\alpha_\sigma(r) = r/\sigma \ \text{ if } \ r \leq 0, \quad \alpha_\sigma(r) = 0 \ \text{ otherwise.}$$

Hence, we readily have that $A : \chi \mapsto (1+\alpha_\sigma)(\chi - \chi_{i-1})/\tau_i$, $-\Delta : H \longrightarrow H$ with domain $D(-\Delta) = W$, and $\beta : H \longrightarrow H$ are all monotone and maximal. Moreover, we readily check that the sum $A - \Delta + \beta$ is maximal monotone and coercive and we apply standard results [7, Cor. 2.7, p. 36] in order to deduce that there exists $\chi_{i,\sigma} \in W$ fulfilling (3.5). As for to remove the σ approximation, we simply refer the reader to [21, Sec. 3] where the limit procedure for $\sigma \to 0$ is fully detailed and we reduce ourselves to a suitable $\chi_i \in W$ fulfilling (3.4).

Now, taking into account the continuous embedding $W \subset L^\infty(\Omega)$, we stress that χ_i is essentially bounded. Thus, we know that $(\chi_i - \chi_{i-1})/\tau_i \in L^\infty(\Omega)$ as well. According to these considerations and the fact that $(\chi_i - \chi_{i-1})/\tau_i \geq 0$ almost everywhere we readily check that

$$M : H \longrightarrow H \qquad M\theta := (1 + (\chi_i - \chi_{i-1}))\theta$$

is positive, linear, and continuous, hence maximal monotone. Rewriting (3.3) as

$$M\theta_i - \tau_i \Delta\theta_i = \theta_{i-1}$$

and arguing as above we conclude the existence part of the Lemma. The uniqueness proof simply follows by contradiction, arguing separately on the two equations (3.3) and (3.4). ☐

Owing to the latter well-posedness result, we are now in the position of exploiting the above introduced notation and rewrite the system (3.3)-(3.4) in the compact form

$$\dot\theta_{\mathcal{P}} + \overline{\theta}_{\mathcal{P}}\,\dot\chi_{\mathcal{P}} - \Delta\overline{\theta}_{\mathcal{P}} = 0 \quad \text{a.e. in } Q, \tag{3.6}$$

$$\dot\chi_{\mathcal{P}} + \overline{\xi}_{\mathcal{P}} - \Delta\overline{\chi}_{\mathcal{P}} + \beta(\overline{\chi}_{\mathcal{P}}) = \mathcal{T}_{\mathcal{P}}\overline{\theta}_{\mathcal{P}} - \theta_c \quad \text{a.e. in } Q, \tag{3.7}$$

$$\overline{\xi}_{\mathcal{P}} \in \alpha(\dot\chi_{\mathcal{P}}) \quad \text{a.e. in } Q. \tag{3.8}$$

4 Stability and Convergence

We shall start from the following unconditional stability result.

Lemma 4.1 (Stability). *Let $\{\theta_i, \chi_i\}_{i=0}^N$ solve (3.2)-(3.4) and $0 \leq \theta_{0\mathcal{P}} \leq \theta_*$ almost everywhere in Ω. Then there exists a constant C_{stab} depending just on Ω, T, θ_*, and j such that*

$$0 \leq \theta_{\mathcal{P}} \leq \theta_* \qquad a.e. \ in \ Q, \tag{4.1}$$

$$\begin{aligned}&\|\theta_{\mathcal{P}}\|_{H^1(0,T;H)\cap L^2(0,T;W)} + \|\chi_{\mathcal{P}}\|_{W^{1,\infty}(0,T;H)\cap H^1(0,T;V)\cap L^\infty(0,T;W)} \\ &\quad + \|\overline{\xi}_{\mathcal{P}}\|_{L^\infty(0,T;H)} \ \leq \ C_{stab}\left(1 + \|\theta_{0\mathcal{P}}\|_V + \|\chi_{0\mathcal{P}}\|_W\right).\end{aligned} \tag{4.2}$$

Moreover, whenever $\theta_{0\mathcal{P}}$, $\chi_{0\mathcal{P}}$ fulfill (2.14) as well, the above constant C_{stab} can be chosen in such a way that

$$\|\tilde{\chi}_{\mathcal{P}}\|_{H^2(0,T;H)} + \|\chi_{\mathcal{P}}\|_{W^{1,\infty}(0,T;V)} \leq C_{stab}\,(1 + \|\theta_{0\mathcal{P}}\|_V + \|\chi_{0\mathcal{P}}\|_W + \|\eta_{0\mathcal{P}}\|_V)\,, \tag{4.3}$$

where we have defined $\eta_{0\mathcal{P}} := (1+\alpha)^{-1}(\Delta\chi_{0\mathcal{P}} - \beta(\chi_{0\mathcal{P}}) + \theta_{0\mathcal{P}} - \theta_c)$.

Proof. Within this proof C will stand for some suitable constant depending on Ω, T, θ_*, and j and possibly varying from line to line.

Let us start from checking the crucial bound (4.1) by induction. Indeed, it suffices to take the product in H of (3.3) and the function $-\theta_i^- = \min\{0, \theta_i\} \in V$ in order to get that

$$\|\theta_i^-\|^2 + (\theta_{i-1}, \theta_i^-) + \tau_i \int_\Omega |\nabla\theta_i^-|^2 = \int_\Omega (\chi_i - \chi_{i-1})\,\theta_i\,\theta_i^- .$$

We now exploit the induction hypothesis $\theta_{i-1} \geq 0$ a.e. in Ω and the essential non-negativity of $\chi_i - \chi_{i-1}$ and obtain

$$\theta_i^- = 0 \quad \text{a.e. in } \Omega \quad \Longrightarrow \quad \theta_i \geq 0 \quad \text{a.e. in } \Omega.$$

Next, we multiply (3.3) by $(\theta_i - \theta_*)^+ := \max\{0, \theta_i - \theta_*\} \in V$ and get

$$\|(\theta_i - \theta_*)^+\|^2 + ((\theta_* - \theta_{i-1}), (\theta_i - \theta_*)^+) + \tau_i \int_\Omega |\nabla((\theta_i - \theta_*)^+)|^2$$
$$= -\int_\Omega (\chi_i - \chi_{i-1})\,\theta_i(\theta_i - \theta_*)^+ .$$

Once again, by using both the induction hypothesis $\theta_{i-1} \leq \theta_*$ a.e. in Ω and the already proved essential non-negativity of θ_i, we conclude for (4.1).

By exploiting the above derived uniform bound on $\theta_{\mathcal{P}}$ we readily deduce the bound in (4.2) by means of standard parabolic estimates techniques. In particular, one multiplies (3.6) by $\dot{\theta}_{\mathcal{P}}$ and (3.7) by $\dot{\chi}_{\mathcal{P}}$, takes the integral on Q_t for $t \in (0,T)$ of the two relations, and makes use of (4.1) in order to get that

$$\int_0^t \|\dot{\theta}_{\mathcal{P}}\|^2 + \frac{1}{2}\int_\Omega |\nabla\theta_{\mathcal{P}}|^2 \leq \frac{1}{2}\int_\Omega |\nabla\theta_{0\mathcal{P}}|^2 + \theta_* \int_0^t \|\dot{\chi}_{\mathcal{P}}\|\,\|\dot{\theta}_{\mathcal{P}}\|, \tag{4.4}$$

$$\int_0^t \|\dot{\chi}_{\mathcal{P}}\|^2 + \frac{1}{2}\int_\Omega \big(|\nabla\chi_{\mathcal{P}}(t)|^2 + j(\chi_{\mathcal{P}}(t))\big)$$
$$\leq \frac{1}{2}\int_\Omega \big(|\nabla\chi_{0\mathcal{P}}|^2 + j(\chi_{0\mathcal{P}})\big) + 2\theta_*|\Omega|^{\frac{1}{2}} \int_0^t \|\dot{\chi}_{\mathcal{P}}\|, \tag{4.5}$$

where $|\Omega|$ stands for the Lebesgue measure of Ω. In the above computations we also exploited the following facts

$$\nabla\overline{\theta}_{\mathcal{P}} \cdot \nabla\dot{\theta}_{\mathcal{P}} \geq \nabla\theta_{\mathcal{P}} \cdot \nabla\dot{\theta}_{\mathcal{P}}, \quad \nabla\overline{\chi}_{\mathcal{P}} \cdot \nabla\dot{\chi}_{\mathcal{P}} \geq \nabla\chi_{\mathcal{P}} \cdot \nabla\dot{\chi}_{\mathcal{P}} \quad \text{a.e. in } Q,$$
$$\text{and} \quad \int_0^t (\beta(\overline{\chi}_{\mathcal{P}}), \dot{\chi}_{\mathcal{P}}) \geq \int_\Omega \big(j(\chi_{\mathcal{P}}(t)) - j(\chi_{0\mathcal{P}})\big).$$

Let us just discuss the first inequality above. Indeed, for all $t \in (t_{i-1}, t_i]$, $i = 1, \ldots, N$, we have that

$$\nabla\overline{\theta}_{\mathcal{P}}(t) \cdot \nabla\dot{\theta}_{\mathcal{P}}(t) = \nabla\theta_{\mathcal{P}}(t) \cdot \nabla\dot{\theta}_{\mathcal{P}}(t) + \big(\nabla\overline{\theta}_{\mathcal{P}}(t) - \nabla\theta_{\mathcal{P}}(t)\big) \cdot \nabla\dot{\theta}_{\mathcal{P}}(t)$$
$$= \nabla\theta_{\mathcal{P}}(t) \cdot \nabla\dot{\theta}_{\mathcal{P}}(t) + \nabla\Big(\theta_i - \gamma_i(t)\theta_i - (1-\gamma_i(t))\theta_{i-1}\Big) \cdot \nabla\left(\frac{\theta_i - \theta_{i-1}}{\tau_i}\right)$$
$$= \nabla\theta_{\mathcal{P}}(t) \cdot \nabla\dot{\theta}_{\mathcal{P}}(t) + \frac{1-\gamma_i(t)}{\tau_i}\,\|\nabla(\theta_i - \theta_{i-1})\|^2 \geq \nabla\theta_{\mathcal{P}}(t) \cdot \nabla\dot{\theta}_{\mathcal{P}}(t) \quad \text{a.e. in } \Omega. \tag{4.6}$$

Hence, taking the sum of (4.4) with a suitable multiple of (4.5) we immediately get that

$$\begin{aligned} &\|\theta_{\mathcal{P}}\|_{H^1(0,T;H)\cap L^\infty(0,T;V)} + \|\chi_{\mathcal{P}}\|_{H^1(0,T;H)\cap L^\infty(0,T;V)} \\ &\quad \leq \; C\left(1+\|\theta_{0\mathcal{P}}\|_V + \|\chi_{0\mathcal{P}}\|_V + \|j(\chi_{0\mathcal{P}})\|_{L^1(\Omega)}\right). \end{aligned} \tag{4.7}$$

Now, by comparison in (3.6) and standard elliptic estimates, we obtain

$$\|\theta_{\mathcal{P}}\|_{L^2(0,T;W)} \; \leq \; C\left(1+\|\theta_{0\mathcal{P}}\|_V + \|\chi_{0\mathcal{P}}\|_V + \|j(\chi_{0\mathcal{P}})\|_{L^1(\Omega)}\right).$$

Next, our second estimate consists in multiplying (3.7) by the function $\partial_t(-\Delta\chi_{\mathcal{P}} + (\beta(\chi))_{\mathcal{P}})$ and exploiting (4.7). Indeed, let us multiply (3.4) by $\tau_i\rho_i$ where

$$\rho_i := -\Delta\eta_i + \zeta_i := -\Delta\left(\frac{\chi_i-\chi_{i-1}}{\tau_i}\right) + \left(\frac{\beta(\chi_i)-\beta(\chi_{i-1})}{\tau_i}\right) \quad \text{for } \; i=1,\ldots,N,$$

and take the integral over Ω obtaining

$$\tau_i(\eta_i,\rho_i) + \tau_i(\xi_i,\rho_i) + \tau_i(-\Delta\chi_i+\beta(\chi_i),\rho_i) = \tau_i(\theta_{i-1}-\theta_c,\rho_i), \tag{4.8}$$

where $\xi_i \in \alpha(\eta_i)$ almost everywhere in Ω. We readily check that

$$\tau_i(\eta_i,\rho_i) = \tau_i\int_\Omega |\nabla\eta_i|^2 + \tau_i(\eta_i,\zeta_i) \geq \tau_i\int_\Omega|\nabla\eta_i|^2,$$

where we simply exploited the monotonicity of β. On the other hand,

$$\tau_i(\xi_i,\rho_i) = -\tau_i(\xi_i,\Delta\eta_i) + (\xi_i,\zeta_i),$$

and the above right hand side is non-negative due to [8, Lemma 2] and the monotonicity of α and β. Finally, we readily check that

$$\tau_i(-\Delta\chi_i+\beta(\chi_i),\rho_i) = \frac{1}{2}\|-\Delta\chi_i+\beta(\chi_i)\|^2 + \frac{\tau_i^2}{2}\|\rho_i\|^2 - \frac{1}{2}\|-\Delta\chi_{i-1}+\beta(\chi_{i-1})\|^2.$$

Next, we take the sum in (4.8) for $i=1,\ldots,m$ $(m\leq N)$. One has that

$$\begin{aligned} &\sum_{i=1}^m \tau_i\int_\Omega|\nabla\eta_i|^2 + \frac{1}{2}\|-\Delta\chi_m+\beta(\chi_m)\|^2 \\ &\leq \frac{1}{2}\|-\Delta\chi_{0\mathcal{P}}+\beta(\chi_{0\mathcal{P}})\|^2 - \sum_{i=1}^m\tau_i(\theta_{i-1}-\theta_c,\rho_i). \end{aligned} \tag{4.9}$$

The second term on the right hand side above may be handled by means of a discrete integration by parts procedure. Namely, we easily infer that

$$\begin{aligned} \sum_{i=1}^m\tau_i(\theta_{i-1}-\theta_c,\rho_i) &= -\sum_{i=1}^{m-1}\tau_i\big((\theta_i-\theta_{i-1})/\tau_i, -\Delta\chi_i+\beta(\chi_i)\big) \\ &+\big(\theta_{m-1}-\theta_c,-\Delta\chi_m+\beta(\chi_m)\big) - \big(\theta_{0\mathcal{P}}-\theta_c,-\Delta\chi_{0\mathcal{P}}+\beta(\chi_{0\mathcal{P}})\big). \end{aligned}$$

Hence, owing to (4.7), we readily apply the discrete Gronwall lemma and obtain that

$$\|\chi_{\mathcal{P}}\|_{H^1(0,T;V)\cap L^\infty(0,T;W)} \; \leq \; C\left(1+\|\theta_{0\mathcal{P}}\|_V + \|j(\chi_{0\mathcal{P}})\|_{L^1(\Omega)} + \|\chi_{0\mathcal{P}}\|_W + \|\beta(\chi_{0\mathcal{P}})\|\right).$$

Finally, the proof of (4.2) follows from a comparison in (3.7) and (2.3).

Let us now turn our attention to the proof of (4.3) under the extra assumption that $\theta_{0\mathcal{P}}$, $\chi_{0\mathcal{P}}$ fulfill (2.14). To this aim, we recall that

$$\eta_{0\mathcal{P}} = (1+\alpha)^{-1}(\Delta\chi_{0\mathcal{P}} - \beta(\chi_{0\mathcal{P}}) + \theta_{0\mathcal{P}} - \theta_c) \in V,$$

so that (3.4) at level 0 reads

$$\eta_{0\mathcal{P}} + \xi_{0\mathcal{P}} - \Delta\chi_{0\mathcal{P}} + \beta(\chi_{0\mathcal{P}}) = \theta_{0\mathcal{P}} - \theta_c, \quad \xi_{0\mathcal{P}} \in \alpha(\eta_{0\mathcal{P}}) \quad \text{a.e. in } \Omega.$$

We now take the difference between relation (3.4) written at level i and the same relation at level $i-1$ for $i = 1, \ldots, N$, multiply the resulting relation by $(\eta_i - \eta_{i-1})/\tau_i$, and take the integral on Ω obtaining (recall (3.1))

$$\begin{aligned}
&\frac{1}{\tau_i}\|\eta_i - \eta_{i-1}\|^2 + \frac{1}{2}\int_\Omega |\nabla\eta_i|^2 - \frac{1}{2}\int_\Omega |\nabla\eta_{i-1}|^2 \\
&\leq \Lambda\,\|\eta_i\|\,\|\eta_i - \eta_{i-1}\| + \frac{1}{\tau_i}\|\theta_i - \theta_{i-1}\|\,\|\eta_i - \eta_{i-1}\|,
\end{aligned}$$

where we also used the monotonicity of α and the Lipschitz continuity of β. Next, taking the sum for $i = 1, \ldots, m$, and exploiting (4.7), we readily get that

$$\frac{1}{2}\sum_{i=1}^{m}\tau_i\left\|\frac{\eta_i - \eta_{i-1}}{\tau_i}\right\|^2 + \frac{1}{2}\int_\Omega |\nabla\eta_m|^2 \leq \frac{1}{2}\int_\Omega |\nabla\eta_{0\mathcal{P}}|^2 + C,$$

and the assertion follows. □

Let us now state the convergence result.

Lemma 4.2. *Let* $\{\theta_i, \chi_i\}_{i=0}^N$ *solve (3.2)-(3.4). Moreover, let*

$$(\theta_{0\mathcal{P}}, \chi_{0\mathcal{P}}) \ \textit{be bounded in} \ V \times W \ \textit{and converge strongly to} \ (\theta_0, \chi_0) \ \textit{in} \ H \times V. \tag{4.10}$$

as the diameter τ *of partition* $\mathcal{P}$ *tends to* 0. *Then, there exists a triplet of functions* (θ, χ, ξ) *such that*

$$\begin{aligned}
\theta_{\mathcal{P}} \longrightarrow \theta \quad & \textit{weakly star in} \ H^1(0,T;H) \cap L^2(0,T;W) \cap L^\infty(Q) \\
& \textit{and strongly in} \ C^0([0,T];H) \cap L^2(0,T;V), && (4.11)\\
\chi_{\mathcal{P}} \longrightarrow \chi \quad & \textit{weakly star in} \ H^1(0,T;V) \cap L^\infty(0,T;W) \cap W^{1,\infty}(0,T;H) \\
& \textit{and strongly in} \ H^1(0,T;H) \cap C^0([0,T];V), && (4.12)\\
\overline{\xi}_{\mathcal{P}} \longrightarrow \xi \quad & \textit{weakly star in} \ L^\infty(0,T;H), && (4.13)
\end{aligned}$$

such that (2.9)-(2.12) are fulfilled. Moreover, as soon as

$$(1+\alpha)^{-1}(\Delta\chi_{0\mathcal{P}} - \beta(\chi_{0\mathcal{P}}) + \theta_{0\mathcal{P}} - \theta_c) \ \textit{are bounded in} \ V, \tag{4.14}$$

we also have that

$$\tilde{\chi}_{\mathcal{P}} \longrightarrow \chi \quad \textit{weakly in} \ H^2(0,T;H), \tag{4.15}$$

$$\chi_{\mathcal{P}} \longrightarrow \chi \quad \textit{weakly star in} \ W^{1,\infty}(0,T;V). \tag{4.16}$$

Proof. Owing to (4.10) we readily find a constant C_{data} such that

$$\|\theta_{0\mathcal{P}}\|_V + \|\chi_{0\mathcal{P}}\|_W \le C_{data},$$

independently of the partition $\mathcal{P}$. Then, thanks to well-known compactness results, estimates (4.1)-(4.2) allows us to find a triplet (θ, χ, ξ) such that, possibly taking not relabeled subsequences, the above stated weak star convergences hold. As for the strong convergences in (4.11) and the strong convergence of $\chi_{\mathcal{P}}$ in $C^0([0,T];V)$ we may exploit [34, Cor. 4]. On the other hand, the strong convergence of $\chi_{\mathcal{P}}$ in $H^1(0,T;H)$ does not follow from compactness arguments and we postpone its proof to Section 5. Moreover, in view of the uniqueness of the solution to the continuous problem, one gets also that the convergences (4.11)-(4.13) hold indeed for the whole sequence as $\tau \to 0$, and not just for a subsequence.

Taking into account (4.2) we have in particular that

$$\|\theta_{\mathcal{P}} - \overline{\theta}_{\mathcal{P}}\|_{L^2(0,T;H)},\ \|\overline{\theta}_{\mathcal{P}} - \mathcal{T}_{\mathcal{P}}\overline{\theta}_{\mathcal{P}}\|^2_{L^\infty(0,T;H)},\ \|\chi_{\mathcal{P}} - \overline{\chi}_{\mathcal{P}}\|_{L^2(0,T;V)} \ \le\ C\tau, \tag{4.17}$$

for some constant C depending on C_{stab} and C_{data}.

Hence, we have that

$$\overline{\theta}_{\mathcal{P}}\,\partial_t\chi_{\mathcal{P}} \longrightarrow \theta\,\partial_t\chi \quad \text{weakly star in } \ L^\infty(0,T;H).$$

The above convergences suffice to write the limit equations (2.9)-(2.10), and to ensure relations (2.6)-(2.8) along with the Cauchy conditions (2.12). Thus, we only have to prove inclusion (2.11). Let us multiply equation (3.7) by $\partial_t\chi_{\mathcal{P}}$ and take the integral over Q. It is straightforward to check that

$$\begin{aligned}\int_0^T\!\!\int_\Omega \overline{\xi}_{\mathcal{P}}\,\partial_t\chi_{\mathcal{P}} &= \int_0^T\!\!\int_\Omega \big(-\partial_t\chi_{\mathcal{P}} - \beta(\overline{\chi}_{\mathcal{P}}) + \Delta\overline{\chi}_{\mathcal{P}} + \mathcal{T}_{\mathcal{P}}\overline{\theta}_{\mathcal{P}} - \theta_c\big)\,\partial_t\chi_{\mathcal{P}}\\ &\le -\|\partial_t\chi_{\mathcal{P}}\|^2_{L^2(0,T;H)} - \int_\Omega j\big(\chi_{\mathcal{P}}(T)\big) + \int_\Omega j\big(\chi_{0\mathcal{P}}\big)\\ &\quad - \int_0^T\!\!\int_\Omega \nabla\overline{\chi}_{\mathcal{P}}\cdot\nabla\partial_t\chi_{\mathcal{P}} + \int_0^T\!\!\int_\Omega (\mathcal{T}_{\mathcal{P}}\overline{\theta}_{\mathcal{P}} - \theta_c)\,\partial_t\chi_{\mathcal{P}}.\end{aligned}$$

Next, we take the $\limsup$ as $\tau \to 0$ on both sides of the latter relation. Of course we have that

$$\limsup_{\tau\to 0} - \int_\Omega j\big(\chi_{\mathcal{P}}(T)\big) = -\liminf_{\tau\to 0}\int_\Omega j\big(\chi_{\mathcal{P}}(T)\big) \le -\int_\Omega j\big(\chi(T)\big), \tag{4.18}$$

where the last inequality holds since $\chi_{\mathcal{P}}$ converges strongly to χ in $C([0,T];V)$. Finally, owing to (2.3) and the strong convergence of $\chi_{0\mathcal{P}}$, it is a standard matter to check that

$$\int_\Omega j(\chi_{0\mathcal{P}}) \longrightarrow \int_\Omega j(\chi_0).$$

Thus, thanks to the above stated convergences and (4.18), we conclude for

$$\begin{aligned}\limsup_{\tau\to 0}\int_0^T\!\!\int_\Omega \overline{\xi}_{\mathcal{P}}\,\partial_t\chi_{\mathcal{P}} &\le -\|\partial_t\chi\|^2_{L^2(0,T;H)} - \int_\Omega j\big(\chi(T)\big) + \int_\Omega j\big(\chi_0\big)\\ &\quad - \int_0^T\!\!\int_\Omega \nabla\chi\cdot\nabla\partial_t\chi + \int_0^T\!\!\int_\Omega (\theta - \theta_c)\,\partial_t\chi.\end{aligned}$$

Recalling (2.10), the right hand side of the previous equation may be rewritten as

$$\int_0^T\int_\Omega \big(- \partial_t\chi - \beta(\chi) + \Delta\chi + \theta - \theta_c\big)\partial_t\chi = \int_0^T\int_\Omega \xi\,\partial_t\chi,$$

hence, one infers that

$$\limsup_{\tau\to 0}\int_0^T\int_\Omega \overline{\xi}_{\mathcal{P}}\,\partial_t\chi_{\mathcal{P}} \le \int_0^T\int_\Omega \xi\,\partial_t\chi.$$

Finally, applying [7, Prop. 2.5, p. 27], relation (2.11) is established.

In case (4.14) holds true, the constant C_{data} above can be chosen in such a way that

$$\|\theta_{0\mathcal{P}}\|_V + \|\chi_{0\mathcal{P}}\|_W + \|\eta_{0\mathcal{P}}\|_V \le C_{data},$$

independently of the partition $\mathcal{P}$. Hence, estimate (4.3) entails that

$$\|\tilde{u}'_{\mathcal{P}} - u'_{\mathcal{P}}\|_{L^2(0,T;H)} \le C\tau,$$

for some constant C depending on C_{stab} and C_{data}. Finally, the proof of the lemma follows from (4.3) and standard compactness arguments. ☐

5 Error control

We now come to the proof of an *a priori* bound of the discretization error.

Lemma 5.1 (Error). *Assume (2.1)-(2.5) and (4.10) and let* $\{\theta_i,\chi_i\}_{i=0}^N$ *solve (3.2)-(3.4) and* (θ,χ,ξ) *fulfill (2.6)-(2.12). Then there exists a positive constant* C_{err} *depending on* C_{stab} *such that*

$$\begin{aligned}\|\theta-\theta_{\mathcal{P}}\|_{C^0([0,T];H)\cap L^2(0,T;V)} &+ \|\chi-\chi_{\mathcal{P}}\|_{H^1(0,T;H)\cap C^0([0,T];V)}\\ &\le C_{err}\Big(\|\theta_0-\theta_{0\mathcal{P}}\| + \|\chi_0-\chi_{0\mathcal{P}}\|_V + \sqrt{\tau}\Big).\end{aligned}\tag{5.1}$$

Proof. Within this proof C stands for any positive constant depending on C_{stab} and may change from line to line. Let us start by fixing two partitions $\mathcal{P}_1, \mathcal{P}_2$ and denote by

$$\mathcal{Q} = \mathcal{P}_1\cup\mathcal{P}_2 = \{0 = q_0 < q_1 < \cdots < q_{M-1} < q_M = T\}.$$

Let now τ_j be the diameter of partition $\mathcal{P}_j$ for $j = 1,2$. Moreover, let us set for the sake of notational convenience

$$(\theta_j,\chi_j) := (\theta_{\mathcal{P}_j},\chi_{\mathcal{P}_j}), \qquad (\overline{\theta}_j,\overline{\chi}_j) := (\overline{\theta}_{\mathcal{P}_j},\overline{\chi}_{\mathcal{P}_j})\quad j = 1,2,$$

and $\hat\theta := \theta_1-\theta_2$, $\hat\chi := \chi_1-\chi_2$ etc.

We take the difference between (3.7) written for $\mathcal{P}_1$ and the same relation for $\mathcal{P}_2$, multiply by $\partial_t\hat\chi$, and integrate on Q_t for $t\in(0,T)$. By exploiting the monotonicity of α one gets

$$\begin{aligned}\int_0^t\int_\Omega \big((\partial_t\hat\chi)^2 + \nabla\hat{\overline{\chi}}\cdot\nabla\partial_t\hat\chi\big) &\le \int_0^t\int_\Omega\Big(- (\beta(\overline{\chi}_1)-\beta(\overline{\chi}_2)) + (\mathcal{T}_{\mathcal{P}_1}\overline{\theta}_1 - \mathcal{T}_{\mathcal{P}_2}\overline{\theta}_2)\Big)\partial_t\hat\chi\\ &\le \frac12\int_0^t\int_\Omega|\partial_t\hat\chi|^2 + \Lambda^2\int_0^t\int_\Omega|\hat{\overline{\chi}}|^2 + \int_0^t\int_\Omega|\mathcal{T}_{\mathcal{P}_1}\overline{\theta}_1 - \mathcal{T}_{\mathcal{P}_2}\overline{\theta}_2|^2,\end{aligned}\tag{5.2}$$

where Λ stands for the actual local Lipschitz constant of β on the ball of suitably big radius $R>0$ depending on C_{stab}, C_{data}, and Ω, and such that $|\chi_j| \le R$ almost everywhere in Q for $j=1,2$.

In order to deal with the latter relation, we compute

$$\int_0^t\int_\Omega \nabla\hat{\overline{\chi}}\cdot\partial_t\nabla\hat\chi = \int_0^t\int_\Omega \nabla\hat\chi\cdot\partial_t\nabla\hat\chi + \int_0^t\int_\Omega \nabla(\hat{\overline{\chi}}-\hat\chi)\cdot\partial_t\nabla\hat\chi.$$

Our aim is to get rid the last *residual* term above. To this end we cannot simply exploit the computation in (4.6) since $\hat\chi$ is not the affine interpolating function of $\hat{\overline{\chi}}$ on the partition $\mathcal{Q}$. By means of (4.2) and (4.17) (the latter will be extensively used throughout this proof), we will simply reason as follows.

$$\int_0^t\int_\Omega \nabla(\hat{\overline{\chi}}-\hat\chi)\cdot\partial_t\nabla\hat\chi \le \|\hat{\overline{\chi}}-\hat\chi\|_{L^2(0,t;V)}\|\partial_t\hat\chi\|_{L^2(0,t;V)} \le C(\tau_1+\tau_2). \tag{5.3}$$

As for the last term in the right hand side on (5.2) we simply exploit (4.17) and deduce that

$$\int_0^t\int_\Omega (\mathcal{T}_{\mathcal{P}_1}\overline\theta_1 - \mathcal{T}_{\mathcal{P}_2}\overline\theta_2)^2 \le \int_0^t\int_\Omega |\hat{\overline\theta}|^2 \ + \ C(\tau_1^2+\tau_2^2).$$

On the other hand, we readily get that

$$\int_0^t\int_\Omega |\hat{\overline\chi}|^2 \le \int_0^t\int_\Omega \left(4s\int_0^s |\partial_t\hat\chi|^2\right) + C\left(\|\hat\chi(0)\|^2+\tau_1^2+\tau_2^2\right).$$

Thus, in particular, relation (5.2) entails

$$\begin{aligned}\int_0^t\int_\Omega |\partial_t\hat\chi|^2 + \|\nabla\hat\chi(t)\|^2 &\le C\int_0^t\int_\Omega \left(4s\int_0^s |\partial_t\hat\chi|^2 ds\right)\\ &\quad + C\left(\|\hat\chi(0)\|_V^2 + \int_0^t\int_\Omega |\hat{\overline\theta}|^2 + \tau_1+\tau_2\right).\end{aligned} \tag{5.4}$$

On the other hand we write the difference between (3.6) written for $\mathcal{P}_1$ and the same relation for $\mathcal{P}_2$ obtaining that

$$\partial_t\hat\theta - \Delta\hat{\overline\theta} = -\overline\theta_1\partial_t\chi_1 + \overline\theta_2\partial_t\chi_2 \quad \text{a.e. in } Q.$$

Now it suffices to multiply the latter relation by $\hat{\overline\theta}$, integrate on Q_t for some $t\in(0,T)$, and recall that $\partial_t\chi_1 \ge 0$ almost everywhere in Q in order to get that

$$\begin{aligned}\int_0^t\int_\Omega \left(\partial_t\hat\theta\,\hat{\overline\theta} + |\nabla\hat{\overline\theta}|^2\right) &= \int_0^t\int_\Omega \left(-\partial_t\chi_1(\hat{\overline\theta})^2 - \overline\theta_2\,\partial_t\hat\chi\,\hat{\overline\theta}\right)\\ \le \theta_*\int_0^t\int_\Omega |\partial_t\hat\chi|\,|\hat{\overline\theta}| &\le \frac14\int_0^t\int_\Omega |\partial_t\hat\chi|^2 + 2\theta_*^2\int_0^t\int_\Omega |\hat\theta|^2 + C(\tau_1^2+\tau_2^2).\end{aligned} \tag{5.5}$$

We shall once again argue as above and deduce that

$$\int_0^t\int_\Omega \partial_t\hat\theta\,\hat{\overline\theta} \ = \ \int_0^t\int_\Omega \partial_t\hat\theta\,\hat\theta + \int_0^t\int_\Omega \partial_t\hat\theta\,(\hat{\overline\theta}-\hat\theta) \ \ge \ \int_0^t\int_\Omega \partial_t\hat\theta\,\hat\theta - C(\tau_1+\tau_2).$$

Hence, taking the sum between (5.4) and (5.5) we readily prove by means of the Gronwall lemma that $\hat\theta$ is a Cauchy sequence in $C^0([0,T];H)\cap L^2(0,T;V)$ and $\hat\chi$ is a Cauchy sequence in $H^1(0,T;H)\cap C^0([0,T];V)$. Moreover, letting for instance the diameter τ_2 go to zero and taking into account the above proved convergences, we readily get that Lemma 5.1 holds. □

As a by-product of the above proof, we have also obtained the strong convergence of $\chi_{\mathcal{P}}$ in $H^1(0,T;H)$. Hence, we are in the position of concluding for Lemma 4.2 as well.

We remark that the convergence rate of estimate (5.1) is sub-optimal with respect to θ since the implicit Euler method was exploited [27, 28]. On the other hand, we do not expect an optimal order of convergence τ with respect to $\dot{\chi}$. Indeed, in the situation of Lemma 5.1, the solution χ may even fail to belong to $H^2(0,T;H)$ (see Lemma 2.4). Finally, no constraint on the possible choice of time-steps has been introduced throughout this analysis. Hence, the time-steps might be tailored according to some further numerical or experimental considerations, possibly including some adaptive procedure.

Acknowledgment. The author would like to acknowledge partial financial support from the NSF and MIUR-COFIN 2002 research program on “Free boundary problems in applied sciences”.

References

[1] D. Blanchard, A. Damlamian, and H. Guidouche. A nonlinear system for phase change with dissipation. *Differential Integral Equations*, 2(3):344–362, 1989.

[2] D. Blanchard and H. Guidouche. A nonlinear system for irreversible phase changes. *European J. Appl. Math.*, 1(1):91–100, 1990.

[3] G. Bonfanti, M. Frémond, and F. Luterotti. Global solution to a nonlinear system for irreversible phase changes. *Adv. Math. Sci. Appl.*, 10(1):1–24, 2000.

[4] G. Bonfanti, M. Frémond, and F. Luterotti. Local solutions to the full model of phase transitions with dissipation. *Adv. Math. Sci. Appl.*, 11(2):791–810, 2001.

[5] G. Bonfanti, M. Frémond, and F. Luterotti. Existence and uniqueness results to a phase transition model based on microscopic accelerations and movements. *Nonlinear Anal. Real World Appl.*, 5(1):123–140, 2004.

[6] G. Bonfanti and F. Luterotti. Convergence results for a phase transition model with vanishing microscopic acceleration. *Math. Models Methods Appl. Sci.*, 14(3):375–392, 2004.

[7] H. Brezis. *Opérateurs maximaux monotones et semi-groupes de contractions dans les espaces de Hilbert*. Number 5 in North Holland Math. Studies. North-Holland, Amsterdam, 1973.

[8] H. Brézis and W. A. Strauss. Semi-linear second-order elliptic equations in L^1. *J. Math. Soc. Japan*, 25:565–590, 1973.

[9] P. Colli, F. Luterotti, G. Schimperna, and U. Stefanelli. Global existence for a class of generalized systems for irreversible phase changes. *NoDEA Nonlinear Differential Equations Appl.*, 9(3):255–276, 2002.

[10] C. M. Dafermos. Global smooth solutions to the initial-boundary value problem for the equations of one-dimensional nonlinear thermoviscoelasticity. *SIAM J. Math. Anal.*, 13(3):397–408, 1982.

[11] C. M. Dafermos and L. Hsiao. Global smooth thermomechanical processes in one-dimensional nonlinear thermoviscoelasticity. *Nonlinear Anal.*, 6(5):435–454, 1982.

[12] M. Frémond. *Non-smooth Thermomechanics*. Springer-Verlag, Berlin, 2002.

[13] M. Frémond and A. Visintin. Dissipation dans le changement de phase. Surfusion. Changement de phase irréversible. *C. R. Acad. Sci. Paris Sér. II Méc. Phys. Chim. Sci. Univers Sci. Terre*, 301(18):1265–1268, 1985.

[14] E. Fried and S. Sellers. Microforces and the theory of solute transport. *Z. Angew. Math. Phys.*, 51(5):732–751, 2000.

[15] M. E. Gurtin. Generalized Ginzburg-Landau and Cahn-Hilliard equations based on a microforce balance. *Phys. D*, 92(3-4):178–192, 1996.

[16] M. E. Gurtin. On the plasticity of single crystals: free energy, microforces, plastic-strain gradients. *J. Mech. Phys. Solids*, 48(5):989–1036, 2000.

[17] P. Krejčí and J. Sprekels. A hysteresis approach to phase-field models. *Nonlinear Anal.*, 39(5, Ser. A: Theory Methods):569–586, 2000.

[18] Ph. Laurençot, G. Schimperna, and U. Stefanelli. Global existence of a strong solution to the one-dimensional full model for irreversible phase transitions. *J. Math. Anal. Appl.*, 271(2):426–442, 2002.

[19] J.-L. Lions and E. Magenes. *Non-homogeneus boundary value problems and applications*, volume 1. Springer-Verlag, New York - Heidelberg, 1972.

[20] F. Luterotti, G. Schimperna, and U. Stefanelli. Existence result for a nonlinear model related to irreversible phase changes. *Math. Models Meth. Appl. Sci.*, 11(5):809–825, 2001.

[21] F. Luterotti, G. Schimperna, and U. Stefanelli. Global solution to a phase field model with irreversible and constrained phase evolution. *Quart. Appl. Math.*, 60(2):301–316, 2002.

[22] F. Luterotti, G. Schimperna, and U. Stefanelli. A generalized phase relaxation model with hysteresis. *Nonlinear Anal.*, 55(4):381–398, 2003.

[23] F. Luterotti and U. Stefanelli. Existence result for the one-dimensional full model of phase transitions. *Z. Anal. Andwendungen*, 21(2):335–350, 2002. Errata & Addendum, *ibid.*, 22(1):239-240, 2002.

[24] A. Miranville. A model of Cahn-Hilliard equation based on a microforce balance. *C. R. Acad. Sci. Paris Sér. I Math.*, 328(12):1247–1252, 1999.

[25] A. Miranville. Generalized Cahn-Hilliard equations based on a microforce balance. *J. Appl. Math.*, (4):165–185, 2003.

[26] A. Miranville and G. Schimperna. Nonisothermal phase separation based on a microforce balance. *Discrete Contin. Dyn. Syst. Ser. B*, 4(3):753-768, 2005.

[27] R. Nochetto, G. Savaré, and C. Verdi. Error control of nonlinear evolution equations. *C. R. Acad. Sci. Paris Sér. I Math.*, 326(12):1437–1442, 1998.

[28] R. Nochetto, G. Savaré, and C. Verdi. A posteriori error estimates for variable time-step discretization of nonlinear evolution equations. *Comm. Pure Appl. Math.*, 53(5):535–589, 2000.

[29] M. Sassetti and A. Tarsia. On a nonlinear vibrating-string equation. *Ann. Mat. Pura Appl. (4)*, 161:1–42, 1992.

[30] G. Schimperna, F. Luterotti, and U. Stefanelli. Local solution to Frémond's full model for irreversible phase transitions. In *Mathematical models and methods for smart materials (Cortona, 2001)*, volume 62 of *Ser. Adv. Math. Appl. Sci.*, pages 323–328. World Sci. Publishing, River Edge, NJ, 2002.

[31] G. Schimperna and U. Stefanelli. Positivity of the temperature for phase transitions with micro-movements. *Nonlinear Anal. Real. World Appl.*, to appear, 2005.

[32] G. Schimperna and U. Stefanelli. A quasi-stationary phase-field model with micro-movements. *Appl. Math. Optim.*, 50(1):67–86, 2004.

[33] G. Savaré. Approximation and regularity of evolution variational inequalities. *Rend. Accad. Naz. Sci. XL Mem. Mat. (5)*, 17:83–111, 1993.

[34] J. Simon. Compact Sets in the Space $L^p(0,T;B)$. *Ann. Mat. Pura Appl. (4)*, 146:65–96, 1987.