Weierstraß–Institut
für Angewandte Analysis und Stochastik

im Forschungsverbund Berlin e.V.

Preprint ISSN 0946 – 8633

A Posteriori Error Estimates for a Time Discrete Scheme for a Phase–Field system of Penrose–Fife type

Olaf Klein [1,*] , Claudio Verdi[2,**]

submitted: September 6, 2001

[1] Weierstrass Institute for Applied Analysis and Stochastics
Mohrenstr. 39
D-10117 Berlin
Germany
E-mail: klein@wias-berlin.de

[2] Dipartimento di Matematica
Università di Milano
Via Saldini 50
I-20133 Milano
Italy
E-mail: verdi@mat.unimi.it

Preprint No. 677
Berlin 2001

2000 *Mathematics Subject Classification.* 65M15, 35K60, 80A22, 35K45.

Key words and phrases. Phase–field model, semidiscretization, a posteriori error estimates.

[*] Partially supported by TMR contracts "Viscosity Solutions and their Applications" and "Asymptotic Methods in Kinetic Theory" and by DFG contract SP 212/10-3

[**] Partially supported by TMR contract "Viscosity Solutions and their Applications" and by MURST Cofin project "Calcolo Scientifico: Modelli e Metodi Numerici Innovativi".

Edited by
Weierstraß–Institut für Angewandte Analysis und Stochastik (WIAS)
Mohrenstraße 39
D — 10117 Berlin
Germany

Fax: + 49 30 2044975
E-Mail (X.400): c=de;a=d400-gw;p=WIAS-BERLIN;s=preprint
E-Mail (Internet): preprint@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

Abstract

A time discrete scheme is used to approximate the solution to a phase field system of Penrose–Fife type with a non–conserved order parameter. An a posteriori error estimate is presented that allows to estimate the difference between continuous and semidiscrete solutions by quantities that can be calculated from the approximation and given data.

1 Introduction

The dynamics of diffusive phase transitions can be described by the evolution of the absolute temperature θ and of an order parameter χ, which characterizes the different phases. In [PF90], Penrose and Fife derived a class of phase field systems, where the evolution of these quantities is determined by an energy balance coupled with a kinetic equation for the order parameter. For a non–conserved order parameter, we consider the following system

$$c_0\theta_t + \lambda'(\chi)\chi_t + \nabla q = g, \quad q = \kappa\nabla\left(\frac{1}{\theta}\right), \tag{1.1a}$$

$$\eta\chi_t - \varepsilon\Delta\chi + s'(\chi) = -\frac{\lambda'(\chi)}{\theta}. \tag{1.1b}$$

In the energy balance (1.1a), the positive constant c_0 represents the specific heat, the function $\lambda'(\chi)$ represents the phase transition latent heat, q represents the heat flux, and the datum g represents heat sources or sinks.

In [PF90], general heat flux laws of the form $\kappa_*(\theta)\nabla(1/\theta)$ have been considered. For $\kappa_*(\theta) = \kappa_0\theta^2$, with $\kappa_0 > 0$ constant, one gets the classical Fourier law. In this framework, we use a constant positive thermal conductivity κ and consider the heat flux law arising for $\kappa_* :\equiv \kappa$, similar to a number of paper where existence and uniqueness of the solution have been investigated [Hor93, HLS96, HSZ96, Kle97, Lau93, Lau95, SZ93, Zhe95]. More general heat flux laws have been considered in [CL98, CLS99, CS98, Kle, Lau98] and [DK97, KK99, KN94].

In the kinetic equation (1.1b), η stands for a positive, space–dependent, kinetic relaxation coefficient, the positive constant ε represents the energy of the phase interfaces, and s' is the derivative of some potential on $\mathbb{R}$.

In the context of a solid–liquid phase transition with a critical temperature θ_C, one typically has a quadratic or linear function λ and the potential $s(r)$ is the sum of $\lambda(r)/\theta_C$ and some other non–convex potential, like, for example, the *double well potential* $(r^2-1)^2$ or the *double obstacle potential* $I_{[-1,1]}(r) + (1-r^2)$. With $I_{[-1,1]}$ being the indicator function of the interval

$[-1,1]$, the latter ensures that the order parameter attains only values in the interval $[-1,1]$. To deal with a general class of potentials, we consider s decomposed as $s = \phi - \sigma$, where ϕ is the convex, but maybe not differentiable, part the the potential, whereas σ represents the not–convex, but differentiable, part of the potential.

In [Hor93], Horn considers a time discrete scheme for a Penrose–Fife system in one space dimension and derives an error estimate of order $\sqrt{h}$, where h denotes the time–step size. In [Kle97, Kle99], the first author of the present paper considers the three dimensional case and prove an error estimate of order h for time discrete schemes. These *a priori* error estimates allow to estimate the order of the error, but can not be used as local refinement error indicators, because they involve non–computable quantities.

In the present paper we investigate a time discrete scheme proposed in [Kle99] and prove an *a posteriori* error estimate. This estimate leads to an upper bound for the difference between the solution to the Penrose–Fife system and its time discrete approximation, which can be calculated using only the given data and the computed solution.

We refer to [NSaV00] and the references quoted therein for the discussion of *a posteriori* error estimates for time evolution problems in a very general framework, which unfortunately does not include our Penrose–Fife model. We refer also to [CNS00, NScV00] for *a posteriori* error estimates and the implementation of adaptive strategies for simpler phase transition models.

The layout of this paper is as follows. In Section 2, the initial–boundary value problem for the phase field system is presented and the time discrete scheme is introduced. The a posteriori error estimates are presented in Section 3. Therein, the result for λ convex is presented first, because the a posteriori error estimate for this case is quite satisfying, whereas the one that holds for general functions λ is somehow weaker. These error estimates are proved in Section 4.

2 The Penrose–Fife system and the time discrete scheme

2.1 The phase–field system

In the sequel, $\Omega \subset \mathbb{R}^N$ with $N = 2, 3$ denotes a bounded open domain with smooth boundary Γ and unit outward normal n. Let $\Omega_T := \Omega \times (0,T)$ and $\Gamma_T := \Gamma \times (0,T)$, where $T > 0$ stands for a final time.

We consider the following initial–boundary value problem for the Penrose–Fife system:

(PF): Find a quadruple (θ, u, χ, ξ) fulfilling

$$\theta \in H^1(0,T;L^2(\Omega)), \quad u \in L^2(0,T;H^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega)), \tag{2.1a}$$

$$\chi \in H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H^2(\Omega)), \tag{2.1b}$$

$$\xi \in L^\infty(0,T;L^2(\Omega)), \tag{2.1c}$$

$$\theta > 0, \quad u = \frac{1}{\theta}, \quad \chi \in D(\beta), \quad \xi \in \beta(\chi), \quad \text{a.e. in} \quad \Omega_T, \tag{2.1d}$$

$$c_0 \frac{\partial \theta}{\partial t} + \lambda'(\chi)\frac{\partial \chi}{\partial t} + \kappa \Delta u = g, \quad \text{a.e. in} \quad \Omega_T, \tag{2.1e}$$

$$\eta \frac{\partial \chi}{\partial t} - \varepsilon \Delta \chi + \xi - \sigma'(\chi) = -\lambda'(\chi) u, \quad \text{a.e. in} \quad \Omega_T, \tag{2.1f}$$

$$\kappa \frac{\partial u}{\partial n} + \gamma u = \zeta, \quad \frac{\partial \chi}{\partial n} = 0, \quad \text{a.e. on} \quad \Gamma_T, \tag{2.1g}$$

$$\theta(\cdot, 0) = \theta^0, \quad \chi(\cdot, 0) = \chi^0, \quad \text{a.e. in} \quad \Omega. \tag{2.1h}$$

As indicated in the first section, c_0, κ, and ε are fixed positive constants, and also γ is one. For dealing with this system, the following assumptions will be used:

(A1) Let β be a maximal monotone graph on $\mathbb{R}$, $\phi : \mathbb{R} \to [0, \infty]$ be a proper lower semicontinuous convex function, and ϕ_1, ϕ_0 be positive constants satisfying

$$\beta = \partial \phi, \quad 0 \in D(\beta), \quad 0 \in \beta(0), \quad \text{int } D(\beta) \neq \emptyset,$$
$$\phi(s) \geq \phi_1 s^2 - \phi_0, \quad \forall\, s \in D(\beta).$$

(A2) There are positive constants $\lambda''_1, \sigma''_1, \sigma'''_1$ and constants $\lambda''_0, \sigma_0 \in \mathbb{R}$, such that

$$\lambda \in W^{2,\infty}_{\text{loc}}(\mathbb{R}), \quad \lambda''_0 \leq \lambda''(s) \leq \lambda''_1, \quad \text{for a.e. } s \in D(\beta),$$
$$\sigma \in W^{3,\infty}_{\text{loc}}(\mathbb{R}), \quad \sigma(s) \leq \frac{1}{4}\phi(s) + \sigma_0, \quad |\sigma''(s)| \leq \sigma''_1, \quad |\sigma'''(s)| \leq \sigma'''_1, \quad \text{for a.e. } s \in D(\beta).$$

(A3) There are positive constants η_0, η_1, and ζ_0 such that

$$\eta \in L^\infty(\Omega), \quad \eta_0 \leq \eta \leq \eta_1, \quad \text{a.e. in} \quad \Omega,$$
$$\zeta \in H^1(0,T;L^2(\Gamma)) \cap L^\infty(\Gamma_T) \cap L^\infty(0,T;H^{1/2}(\Gamma)), \quad \zeta \geq \zeta_0, \quad \text{a.e. on} \quad \Gamma_T,$$
$$g \in H^1(0,T;L^\infty(\Omega)).$$

(A4) Let the initial data $\theta^0, \chi^0, u^0, \xi^0$ satisfy

$$\theta^0, u^0 \in H^1(\Omega) \cap L^\infty(\Omega), \quad \theta^0 > 0, \quad u^0 = \frac{1}{\theta^0}, \quad \text{a.e. in} \quad \Omega,$$
$$\chi^0 \in H^2(\Omega), \quad \xi^0 \in L^2(\Omega), \quad \phi(\chi^0) \in L^1(\Omega), \quad \chi^0 \in D(\beta), \quad \xi^0 \in \beta(\chi^0), \quad \text{a.e. in} \quad \Omega,$$
$$\frac{\partial \chi^0}{\partial n} = 0, \quad \text{a.e. on} \quad \Gamma.$$

From Theorem 2.2 in [Kle99] it follows that, under the assumptions **(A1)**–**(A4)**, there is a unique solution (θ, u, χ, ξ) to the Penrose–Fife system **(PF)**. For this solution it holds that

$$\theta \in L^\infty(0,T;H^1(\Omega)) \,\cap\, L^\infty(\Omega_T) \,\cap\, W^{1,\infty}(0,T;H^1(\Omega)^*), \tag{2.2a}$$

$$u \in H^1(0,T;L^2(\Omega)) \,\cap\, L^\infty(\Omega_T), \tag{2.2b}$$

$$\chi \in W^{1,\infty}(0,T;L^2(\Omega)) \,\cap\, H^1(0,T;H^1(\Omega)) \,\cap\, L^\infty(\Omega_T). \tag{2.2c}$$

2.2 The time discrete scheme

We introduce a time discrete scheme with variable time–steps. Let us consider a partition of the time interval $[0,T]$

$$\mathcal{P} := \{0 = t_0 < t_1 < \cdots < t_M = T\}$$

with variable step

$$h_m := t_m - t_{m-1}, \quad \forall\, m = 1, \dots, M,$$

that satisfies the following assumption:

(A5) There exist two positive constants $c_* \le 1 \le c^*$ such that

$$c_* h_{m-1} \le h_m \le c^* h_{m-1}, \quad \forall\, m = 2, \dots, M,$$

$$h_m < \frac{\min(\eta_0, \phi_1)}{3\sigma_1''}, \quad \forall\, m = 1, \dots, M.$$

Let $h := \max_{1\le m\le M} h_m$ denote the maximum of the time step sizes. For $m = 1, \dots, M$, let

$$g_m(\cdot) := \frac{1}{h_m} \int_{t_{m-1}}^{t_m} g(\cdot,t)\,\mathrm{d}t\,, \quad \text{a.e. in} \quad \Omega, \quad \zeta_m(\cdot) := \frac{1}{h_m} \int_{t_{m-1}}^{t_m} \zeta(\cdot,t)\,\mathrm{d}t\,, \quad \text{a.e. on} \quad \Gamma, \tag{2.3}$$

and let Ω_m denote the cylinder $\Omega_m := \Omega \times (0, t_m)$.

Our Euler scheme in time for the Penrose–Fife systems is implicit, except for the treatment of the nonlinearities λ' and σ', and reads as follows:

(D): Let

$$\theta_0 := \theta^0, \quad u_0 := u^0, \quad \chi_0 := \chi^0, \quad \xi_0 := \xi^0, \tag{2.4a}$$

and, for $m = 1, \dots, M$, find

$$\theta_m \in L^2(\Omega), \quad u_m, \chi_m \in H^2(\Omega), \quad \xi_m \in L^2(\Omega), \tag{2.4b}$$

such that, given g_m and ζ_m as in (2.3),

$$\theta_m > 0, \quad u_m = \frac{1}{\theta_m}, \quad \chi_m \in D(\beta), \quad \xi_m \in \beta(\chi_m), \quad \text{a.e. in} \quad \Omega, \tag{2.4c}$$

$$c_0 \frac{\theta_m - \theta_{m-1}}{h_m} + \lambda'(\chi_{m-1}) \frac{\chi_m - \chi_{m-1}}{h_m} + \kappa \Delta u_m = g_m, \quad \text{a.e. in} \quad \Omega, \tag{2.4d}$$

$$\begin{aligned} &\eta \frac{\chi_m - \chi_{m-1}}{h_m} - \varepsilon \Delta \chi_m + \xi_m - \sigma''(\chi_{m-1})\chi_m \\ &\quad = -\lambda'(\chi_{m-1}) u_m - \sigma''(\chi_{m-1})\chi_{m-1} + \sigma'(\chi_{m-1}), \quad \text{a.e. in} \quad \Omega, \end{aligned} \tag{2.4e}$$

$$-\kappa \frac{\partial u_m}{\partial n} = \gamma u_m - \zeta_m, \quad \frac{\partial \chi_m}{\partial n} = 0, \quad \text{a.e. on} \quad \Gamma. \tag{2.4f}$$

The scheme **(D)** belongs to the class of schemes considered in [Kle99]. Hence, we get from the Corollary 2.1 and Remark 2.2 therein that **(D)** has a unique solution, provided **(A1)**–**(A5)** are satisfied.

Remark 2.1. The assumption **(A5)** is not used in the derivation of the a posteriori error estimates, but to ensure the existence of a unique solution to **(D)**. Hence, in the corollary and the theorems in the next section, the assumption **(A5)** could be replaced by the assumption that a solution to the scheme **(D)** is given. In this case, assumption **(A5)** would have to be added in Remarks 3.4 and 3.10, since therein one is using the uniform upper bounds for the approximations that are proved in [Kle99] under this assumption.

Remark 2.2. The approximation for $\sigma'(\chi)$ used in (2.4e) is linear in χ_m and involves a truncation error with respect to the implicit term $\sigma'(\chi_m)$ bounded by $\sigma_1'''(\chi_m - \chi_{m-1})^2/2$. This approximation coincides with $\sigma'(\chi_m)$ if σ is a quadratic function and σ' is therefore an affine function. In this case, also the lower bound $c_* h_{m-1}$ for h_m in **(A5)** could be skipped, see Remark 2.9 in [Kle99].

We use the solution to **(D)** to construct approximations of the solution to the Penrose–Fife system **(PF)**. The piecewise linear in time function $\widehat{\theta} \in H^1([0,T]; L^2(\Omega))$ is defined by

$$\widehat{\theta}(t) := \theta_{m-1} + \frac{t - t_{m-1}}{h_m}(\theta_m - \theta_{m-1}) \quad \forall\, t \in (t_{m-1}, t_m], \ m = 1, \ldots, M; \tag{2.5}$$

the function $\widehat{\chi} \in H^1(0,T; H^2(\Omega))$ is analogously defined. Moreover, the piecewise constant in time functions $\overline{\chi}$, $\underline{\chi} \in L^\infty(0,T; H^2(\Omega))$ are defined by

$$\overline{\chi}(0) = \underline{\chi}(0) := \chi_0, \quad \overline{\chi}(t) := \chi_m, \quad \underline{\chi}(t) := \chi_{m-1}, \quad \forall\, t \in (t_{m-1}, t_m], \ m = 1, \ldots, M; \tag{2.6}$$

$\overline{u}$, $\underline{u} \in L^\infty(0,T; H^2(\Omega))$ and any piecewise constant function are defined analogously.

3 A posteriori error estimates

3.1 Preliminary notations

Before the a posteriori error estimates can be presented, some notations has to be fixed.

We denote by V the Hilbert space $H^1(\Omega)$ with the inner product $(\cdot,\cdot)_V$ defined by

$$(w,v)_V := \kappa \int_\Omega \nabla w \cdot \nabla v \, \mathrm{d}x \, + \gamma \int_\Gamma wv \, \mathrm{d}\nu \,, \quad \forall\, w,v \in H^1(\Omega), \tag{3.1}$$

and the corresponding norm $\|\cdot\|_V$. Thanks to the trace theorem and Poincaré's inequality, we see that the norms $\|\cdot\|_V$ and $\|\cdot\|_{H^1(\Omega)}$ are equivalent. Hence, V^* can be identified with $H^1(\Omega)^*$ with equivalent norms. Identifying $L^2(\Omega)$ and $L^2(\Gamma)$ with their dual spaces, we can therefore embed both spaces in V^*. There is some positive constant C_*, such that

$$\|w+\psi\|_{V^*} \le C_* \|w\|_{L^2(\Omega)} + \frac{1}{\gamma} \|\psi\|_{L^2(\Gamma)} \,, \quad \forall\, w \in L^2(\Omega),\, \psi \in L^2(\Gamma). \tag{3.2}$$

Following the definition of coercivity for angle bounded operators introduced in [NSaV00, Chap. 4.2], we define $\alpha : (0,\infty)^3 \to [0,\infty)$ by

$$\alpha(v,r,w) := (r-v)\Big(\frac{1}{w}-\frac{1}{r}\Big) + (v-w)\Big(\frac{1}{w}-\frac{1}{v}\Big), \quad \forall\, v,r,w>0. \tag{3.3}$$

Using the piecewise linear function $l : [0,T] \to [0,1]$ defined by

$$l(0) := 0, \qquad l(t) := \frac{t-t_{m-1}}{h_m}, \quad \forall\, t \in (t_{m-1},t_m],\ m=1,\ldots,M, \tag{3.4}$$

and recalling (2.6) and (2.5), one can rewrite the piecewise linear interpolants in the form

$$\widehat{\chi}(t) = l(t)\overline{\chi}(t) + (1-l(t))\underline{\chi}(t), \quad \widehat{\theta}(t) = l(t)\frac{1}{\overline{u}(t)} + (1-l(t))\frac{1}{\underline{u}(t)}, \quad \forall\, t \in [0,T]. \tag{3.5}$$

Finally, for $m=1,\ldots,M$, we set

$$\delta\chi_m := \chi_m - \chi_{m-1}, \quad \delta u_m := u_m - u_{m-1}, \quad \delta\phi_m := \phi(\chi_m) - \phi(\chi_{m-1}). \tag{3.6}$$

3.2 A posteriori error estimates for λ convex

For Penrose–Fife phase field systems with a convex function λ, two a posteriori error estimates are presented. The first one in the corollary below is a direct consequence of the one in the theorem afterwards, but it is presented first because it is less technical than the one in the theorem, whereas the one in the theorem is sharper.

Corollary 3.1. *If (A1)–(A5) and $\lambda_0'' \geq 0$ hold, we have for $k = 1, \dots, M$:*

$$\max\Big\{ \Big\| c_0\theta(t_k) + \lambda(\chi(t_k)) - \big(c_0\widehat{\theta}(t_k) + \lambda(\widehat{\chi}(t_k))\big) \Big\|_{V^*}, \big\| \sqrt{\eta}\,(\chi(t_k) - \widehat{\chi}(t_k)) \big\|_{L^2(\Omega)},$$
$$\min_{0\le m\le k} \psi_{k,m}\Big[\sqrt{2c_0}\Big(\Big\| l\frac{(u-\overline{u})^2}{u\overline{u}} \Big\|_{L^1(\Omega_k)} + \|(1-l)\alpha(\overline{u},u,\underline{u})\|_{L^1(\Omega_k)} \Big)^{1/2}$$
$$+ \sqrt{\varepsilon}\Big(\|\nabla(\chi-\overline{\chi})\|^2_{(L^2(\Omega_k))^N} + \|\nabla(\chi-\widehat{\chi})\|^2_{(L^2(\Omega_k))^N} \Big)^{1/2} \Big] \Big\}$$
$$\leq \Big(\sum_{m=1}^{k} h_m \mathcal{E}_{1,m} \max(\psi^2_{k,m-1}, \psi^2_{k,m}) \Big)^{1/2}$$
$$+ \sum_{m=1}^{k} h_m (\mathcal{E}_{2,m} + \mathcal{E}_{3,m} + \mathcal{E}_{4,m}) \max(\psi_{k,m-1}, \psi_{k,m}), \tag{3.7}$$

with

$$\psi_{k,m} := \exp\Big(\frac{\sigma_1''}{\eta_0}(t_k - t_m) - \frac{\lambda_0''}{2\eta_1} \sum_{i=m+1}^{k} h_i \min_{x\in\overline{\Omega}} u_i(x) \Big), \quad \forall\, m = 0,\dots,k, \tag{3.8}$$

and error indicators $\mathcal{E}_{1,m},\dots,\mathcal{E}_{4,m} \in \mathbb{R}$, which, for $m = 1,\dots,M$, are defined by

$$\mathcal{E}_{1,m} := 2\,\|\xi_m\delta\chi_m - \delta\phi_m\|_{L^1(\Omega)} + \frac{2\varepsilon}{3}\,\|\nabla\delta\chi_m\|^2_{(L^2(\Omega))^N} + 2c_0 \Big\| \frac{(\delta u_m)^2}{u_m u_{m-1}} \Big\|_{L^1(\Omega)}, \tag{3.9a}$$

$$\mathcal{E}_{2,m} := \frac{1}{h_m} C_* \lambda_1'' \,\|\delta\chi_m\|^2_{L^4(\Omega)}, \tag{3.9b}$$

$$\mathcal{E}_{3,m} := \frac{1}{\sqrt{\eta_0}} \Big(\sigma_1''\,\|\delta\chi_m\|_{L^2(\Omega)} + \frac{\sigma_1'''}{3}\,\|\delta\chi_m\|^2_{L^4(\Omega)} + \lambda_1''\,\|u_m\delta\chi_m\|_{L^2(\Omega)} \Big), \tag{3.9c}$$

$$\mathcal{E}_{4,m} := \frac{2}{h_m} \int_{t_{m-1}}^{t_m} \Big(\|g(t) - g_m\|_{V^*} + \frac{1}{\gamma}\,\|\zeta(t) - \zeta_m\|_{L^2(\Gamma)} \Big)\,\mathrm{d}t\,. \tag{3.9d}$$

Remark 3.2. Using the notation $\sum_{i=l}^{k} \dots = 0$ with $l > k$, we note that $\psi_{k,k} = 1$ in (3.8).

The factor $\psi_{k,m}$ indicates in which way the error in the interval $(t_{k-1}, t_k]$ is affected by the approximation in the previous intervals $(t_{m-1}, t_m]$ for $m = 1,\dots,k$. We see that this contribution in increased by the non–convex part σ of the potential, but also reduced by the convexity of λ.

While these factors depend on k and m, the error indicators $\mathcal{E}_{1,m},\dots,\mathcal{E}_{4,m}$ are independent of k. The error indicator $\mathcal{E}_{1,m}$ is related to the approximations of the nonlinearities $\beta(\chi)$ and $1/\theta$ and of the $\Delta\chi$–term in the order parameter equation. The indicator $\mathcal{E}_{2,m}$ measures the effects of using the approximation $\lambda'(\chi_{m-1})(\chi_m - \chi_{m-1})$ in the discrete energy balance (2.4d) instead of $\lambda(\chi_m) - \lambda(\chi_{m-1})$, whereas $\mathcal{E}_{3,m}$ consists of the contributions to the error caused by the approximations of $\sigma'(\chi)$ and $\lambda'(\chi)u$ in the order parameter equation (2.4e). Finally, the error indicator $\mathcal{E}_{4,m}$ is relates to data approximation.

Remark 3.3. Similarly to [Kle97, Kle99], one can use the $L^1(\Omega_T)$–norm of $l(u-\overline{u})^2/u\overline{u}$ and the generalized Hölder's inequality, to derive both $L^2(0,T;L^{3/2}(\Omega))$ and $L^2(\Omega_T)$ estimates for $l(u-\overline{u})$ and $L^1(\Omega_T)$ and $L^2(\Omega_T)$ estimates for $l(\theta-\widehat{\theta})$. But, in addition to norms of $\overline{u}$, $\widehat{\theta}$, and $\widehat{\theta}-1/\overline{u}$, one would also need in this estimates the $L^\infty(0,T;L^6(\Omega))$ and $L^\infty(\Omega_T)$ norms of u and the $L^2(\Omega_T)$ and $L^\infty(\Omega_T)$ norms of θ. Moreover, the linear factor l vanishing as $t\downarrow t_m$, one would have to use the estimate for $(1-l)\alpha(\overline{u},u,\underline{u})$ in the interval $(t_m,t_m+\delta)$ for $\delta>0$ small, to get informations about the approximation error of u.

We note that

$$\alpha(\overline{u},u,\overline{u})=\frac{(u-\overline{u})^2}{u\overline{u}},$$

but unfortunately $\alpha(\overline{u},u,\underline{u})$ is not equal to $\alpha(\overline{u},u,\overline{u})$ in general. Instead, we have to use the following estimates from below for $\alpha(\overline{u},u,\underline{u})$. We get from definition (3.3) that, for all $r,v,w>0$,

$$\alpha(v,r,w)=\frac{(r-v)^2}{rv}+\frac{(v-w)(r-w)}{vw}=\frac{(r-w)^2}{rw}+\frac{(v-w)(v-r)}{vr}, \tag{3.10}$$

$$2\alpha(v,r,w)=\frac{(r-v)^2}{rv}+\frac{(r-w)^2}{rw}+\frac{(v-w)(r-w)^2+w(v-w)^2}{rvw}. \tag{3.11}$$

Arguing by contradiction, from identities (3.10) we infer that

$$\alpha(\overline{u},u,\underline{u})\geq\min\Big(\frac{(u-\overline{u})^2}{u\overline{u}},\frac{(u-\underline{u})^2}{u\underline{u}}\Big),$$

whereas, if $\underline{u}\leq\overline{u}$, (3.11) implies

$$\alpha(\overline{u},u,\underline{u})\geq\frac{1}{2}\frac{(u-\overline{u})^2}{u\overline{u}}+\frac{1}{2}\frac{(u-\underline{u})^2}{u\underline{u}}. \tag{3.12}$$

Considering for $w>v>0$ and $r>0$ the last term in (3.11), we see that it is non–negative if and only if $(r-w)^2\leq w(w-v)$. Hence, we conclude that for $\underline{u}>\overline{u}$ the inequality (3.12) holds if and only if $\underline{u}-\sqrt{\underline{u}(\underline{u}-\overline{u})}\leq u\leq\underline{u}+\sqrt{\underline{u}(\underline{u}-\overline{u})}$.

Remark 3.4. Using the a priori estimates for the semidiscrete solution derived in [Kle99, Chap. 4] and **(A3)**, we see that the $|\psi_{k,m}|$ are uniformly bounded from above and below and that

$$\Big(\sum_{m=1}^{M}h_m\mathcal{E}_{1,m}\Big)^{1/2}+\sum_{m=1}^{M}h_m\Big(\mathcal{E}_{2,m}+\mathcal{E}_{3,m}+\mathcal{E}_{4,m}\Big)\leq Ch,$$

with some constant independent of the partition $\mathcal{P}$ of $[0,T]$. Applying also the regularity results (2.1a)–(2.1c) and (2.2) of the solution, one can recover the a priori error estimate derived in [Kle99, Theorem 2.3], namely there exists a positive constant C, such that for all partition $\mathcal{P}$ satisfying **(A5)**, we have

$$\begin{aligned}\|\widehat{\theta}-\theta\|_{L^2(\Omega_T)\cap C([0,T];H^1(\Omega)^*)}&+\|\widehat{u}-u\|_{L^2(\Omega_T)}\\&+\|\widehat{\chi}-\chi\|_{C([0,T],L^2(\Omega))\cap L^2(0,T;H^1(\Omega))}\leq Ch.\end{aligned} \tag{3.13}$$

Now, the stronger version of the a posteriori error estimate for phase field systems with λ convex is presented.

Theorem 3.5. *If (A1)–(A5) and $\lambda_0'' \geq 0$ hold, we have for $k = 1, \dots, M$:*

$$\max\Big\{ \Big\|\Psi_k\Big(c_0\theta + \lambda(\chi) - \big(c_0\widehat{\theta} + \lambda(\widehat{\chi})\big)\Big)\Big\|_{C([0,t_k];V^*)}, \ \|\Psi_k\sqrt{\eta}\,(\chi - \widehat{\chi})\|_{C([0,t_k];L^2(\Omega))},$$
$$\sqrt{2c_0}\Big(\Big\|\Psi_k^2 l\frac{(u-\overline{u})^2}{u\overline{u}}\Big\|_{L^1(\Omega_k)} + \big\|\Psi_k^2(1-l)\alpha(\overline{u}, u, \underline{u})\big\|_{L^1(\Omega_k)}\Big)^{1/2}$$
$$+ \sqrt{\varepsilon}\Big(\|\Psi_k\nabla(\chi-\overline{\chi})\|^2_{(L^2(\Omega_k))^N} + \|\Psi_k\nabla(\chi-\widehat{\chi})\|^2_{(L^2(\Omega_k))^N}\Big)^{1/2}\Big\}$$
$$\leq \Big(\sum_{m=1}^{k} h_m\mathcal{E}_{1,m}\max(\psi^2_{k,m-1}, \psi^2_{k,m})\Big)^{1/2}$$
$$+ \sum_{m=1}^{k} h_m(\mathcal{E}_{2,m} + \mathcal{E}_{3,m} + \mathcal{E}_{4,m})\max(\psi_{k,m-1}, \psi_{k,m}), \qquad (3.14)$$

with $\psi_{k,m}$, $\mathcal{E}_{1,m}, \dots, \mathcal{E}_{4,m}$ as in Corollary 3.1 and

$$\Psi_k(t) := \exp\Big(\frac{\sigma_1''}{\eta_0}(t_k - t) - \frac{\lambda_0''}{2\eta_1}\Big((t_m - t)\min_{x\in\overline{\Omega}} u_m(x) + \sum_{i=m+1}^{k} h_i \min_{x\in\overline{\Omega}} u_i(x)\Big)\Big),$$
$$\forall\, t \in (t_{m-1}, t_m],\ m = 1, \dots, k. \qquad (3.15)$$

Remark 3.6. For $t \leq t_k$, $\Psi_k(t)$ indicates how much the error at the time t is over– or under–estimated by using the error estimate for the interval $[0, t_k]$. We have $\Psi_k(t_m) = \psi_{k,m}$ for all $m = 0, \dots, k$. Considering the definition (3.15) of Ψ_k, we see that Ψ_k attains its extrema in $[t_{m-1}, t_m]$ at the boundary of this interval. Hence, we see that

$$\min(\psi_{k,m-1}, \psi_{k,m}) \leq \Psi_k(t) \leq \max(\psi_{k,m-1}, \psi_{k,m}), \quad \forall\, t \in [t_{m-1}, t_m],\ m = 1, \dots k. \quad (3.16)$$

Remark 3.7. Damlamian and Kenmochi derived in [DK97] a formulation for the Penrose–Fife system with convex λ that leads to an evolution equation with the subdifferential of some convex, lower semicontinuous functional on $V^* \times L^2(\Omega)$. In the light of this formulation, one could also apply the abstract result in [NSaV00] directly. This result leads to an a posteriori error estimates for a fully implicit time discrete scheme, whose numerical solution would be quite more complicated to implement. Moreover, if λ is not convex, the abstract results of [NSaV00] can not be applied directly, at least not without using quite strong additional assumptions on the solution.

3.3 A posteriori error estimates for general λ

In the system originally considered by Penrose and Fife in [PF90], the function λ was concave. Hence, even if more general λ's are interesting in applications, we see that it is important to have an a posteriori estimate also if λ is not convex. The function Υ_k appearing on the left–hand side of the estimates is now bounded from below by 1. Therefore, in contrast to the situation for the convex λ, no separate corollary without this function is presented.

Theorem 3.8. *Assume that (A1)–(A5) holds. Let $C_\varepsilon > 0$ be a constant, such that*

$$\|v\|_{L^3(\Omega)} \le \sqrt{\varepsilon}\,\|\nabla v\|_{(L^2(\Omega_T))^N} + C_\varepsilon\,\|v\|_{L^2(\Omega)}\,, \quad \forall\, v \in H^1(\Omega). \tag{3.17}$$

Hence, we have for $k = 1,\dots,M$:

$$\begin{aligned}
\max\Big\{ &\Big\|\Upsilon_k\Big(c_0\theta + \lambda(\chi) - \big(c_0\widehat{\theta} + \lambda(\widehat{\chi})\big)\Big)\Big\|_{C([0,t_k];V^*)}\,,\ \|\Upsilon_k\sqrt{\eta}\,(\chi - \widehat{\chi})\|_{C([0,t_k];L^2(\Omega))}\,,\\
&\sqrt{2c_0}\Big(\Big\|\Upsilon_k^2 l\frac{(u-\overline{u})^2}{u\overline{u}}\Big\|_{L^1(\Omega_k)} + \big\|\Upsilon_k^2(1-l)\alpha(\overline{u},u,\underline{u})\big\|_{L^1(\Omega_k)}\Big)^{1/2}\\
&\qquad + \sqrt{\varepsilon}\Big(\|\Upsilon_k\nabla(\chi-\overline{\chi})\|^2_{(L^2(\Omega_k))^N} + \frac{1}{2}\|\Upsilon_k\nabla(\chi-\widehat{\chi})\|^2_{(L^2(\Omega_k))^N}\Big)^{1/2}\Big\}\\
&\le \Big(\sum_{m=1}^{k} h_m\mathcal{E}_{1,m}\upsilon_{k,m}^2\omega_{k,m}^2\exp\Big(2\frac{\sigma_1''}{\eta_0}(t_k - t_{m-1})\Big)\Big)^{1/2}\\
&\quad + \sum_{m=1}^{k} h_m(\mathcal{E}_{4,m} + \mathcal{E}_{5,m} + \mathcal{E}_{6,m})\upsilon_{k,m}\omega_{k,m}\exp\Big(\frac{\sigma_1''}{\eta_0}(t_k - t_{m-1})\Big),
\end{aligned} \tag{3.18}$$

with, for $m = 1,\dots,k$,

$$\begin{aligned}
\Upsilon_k(t) := \exp\Big(&\frac{\sigma_1''}{\eta_0}(t_k - t) + \frac{1}{4\eta_0}\,|\lambda_0''|\,(t_m - t)\,\|u_m\|_{L^6(\Omega)}\,\big(2C_\varepsilon + |\lambda_0''|\,\|u_m\|_{L^6(\Omega)}\big)\\
&+ \frac{1}{4\eta_0}\,|\lambda_0''|\sum_{i=m+1}^{k} h_i\,\|u_i\|_{L^6(\Omega)}\,\big(2C_\varepsilon + |\lambda_0''|\,\|u_i\|_{L^6(\Omega)}\big)\Big), \quad \forall\, t \in (t_{m-1}, t_m],
\end{aligned} \tag{3.19}$$

$$\upsilon_{k,m} := \exp\Big(\frac{1}{2\eta_0}\,|\lambda_0''|\sum_{i=m}^{k} h_i\,\|u_i\|_{L^6(\Omega)}\,\big(C_\varepsilon + |\lambda_0''|\,\|u_i\|_{L^6(\Omega)}\big)\Big), \tag{3.20}$$

$$\omega_{k,m} := \exp\Big(\frac{1}{2\eta_0}\,|\lambda_0''|\int_{t_{m-1}}^{t_k}\|u(\tau)\|_{L^6(\Omega)}\,\big(C_\varepsilon + |\lambda_0''|\,\|u(\tau)\|_{L^6(\Omega)}\big)\,\mathrm{d}\tau\Big), \tag{3.21}$$

error indicators $\mathcal{E}_{1,m}, \mathcal{E}_{4,m}$ as in Corollary 3.1, and error indicators $\mathcal{E}_{5,m}, \mathcal{E}_{6,m}$ which, for $m = 1,\dots,M$, are defined by

$$\mathcal{E}_{5,m} := \frac{1}{h_m}C_*\max\big(|\lambda_0''|\,,\lambda_1''\big)\,\|\delta\chi_m\|^2_{L^4(\Omega)}\,, \tag{3.22a}$$

$$\mathcal{E}_{6,m} := \frac{1}{\sqrt{\eta_0}}\Big(\sigma_1''\,\|\delta\chi_m\|_{L^2(\Omega)} + \frac{\sigma_1'''}{3}\,\|\delta\chi_m\|^2_{L^4(\Omega)} + \max\big(|\lambda_0''|\,,\lambda_1''\big)\,\|u_m\delta\chi_m\|_{L^2(\Omega)}\Big). \tag{3.22b}$$

Remark 3.9. For $t \le t_k$, $\Upsilon_k(t)$ gives a lower bound on the over–estimation of error at the time t by using the error estimate for the interval $[0, t_k]$. There is a function which would estimate this over–estimation better, but this function would require to use informations from the solution u. By the factor $\upsilon_{k,m}\omega_{k,m}\exp((\sigma_1''/\eta_0)(t_k - t_{m-1}))$ it is measured how the error and the contributions to the error corresponding to the time–interval $(t_{m-1}, t_m]$ are increasing the error in the time–interval $(t_{k-1}, t_k]$, because of the non–convex part of the potential and the concavity of λ. The error indicator $\mathcal{E}_{5,m}$ coincides with $\mathcal{E}_{2,m}$ if $|\lambda_0''| \le \lambda_1''$. Both indicators measure the same kind of contribution to the error. The error indicators $\mathcal{E}_{3,m}$ and $\mathcal{E}_{6,m}$ are related likewise.

Remark 3.10. Similar as in Remark 3.4, we see that the $|v_{k,m}|$ are uniformly bounded from above and that

$$\Big(\sum_{m=1}^{M} h_m \mathcal{E}_{1,m}\Big)^{1/2} + \sum_{m=1}^{M} h_m \Big(\mathcal{E}_{4,m} + \mathcal{E}_{5,m} + \mathcal{E}_{6,m}\Big) \le Ch,$$

with some constant independent of the partition $\mathcal{P}$ of $[0,T]$. Since the regulatity (2.2b) of the solution to **(PF)** also yields that there is a uniform upper bound for $\omega_{k,m}$, we conclude that also for general λ the error estimate (3.13) can be recovered from the a posteriori error esimates.

Remark 3.11. A heuristic estimate of the $L^2(0,T;L^6(\Omega))$–norm of u and therefore for $\omega_{k,m}$ can be derived from the fact that by [Kle99, (2.14)–(2.16), (6.3), and (6.8)] and a generalized version of the Aubin Lemma (see [Sim87, Corollary 4]), $\overline{u}$ tends to u strongly in $L^2(0,T;H^1(\Omega))$, if h tends to 0. Thanks to the embedding of $H^1(\Omega)$ in $L^6(\Omega)$, we have therefore for h sufficiently small:

$$\omega_{k,m} \le 2 v_{k,m}, \quad \forall\, m = 1, \ldots, k. \tag{3.23}$$

If this estimate holds, we can estimate the right–hand side of (3.18) by

$$\begin{aligned} &2\Big(\sum_{m=1}^{k} h_m \mathcal{E}_{1,m} v_{k,m}^4 \exp\Big(2\frac{\sigma_1''}{\eta_0}(t_k - t_{m-1})\Big)\Big)^{1/2} \\ &\quad + 2\sum_{m=1}^{k} h_m (\mathcal{E}_{4,m} + \mathcal{E}_{5,m} + \mathcal{E}_{6,m}) v_{k,m}^2 \exp\Big(\frac{\sigma_1''}{\eta_0}(t_k - t_{m-1})\Big), \end{aligned}$$

and get a computable a posteriori error estimate, which only involves the computed approximation, some data, and the error in the approximation of the data.

Since one can not ensure that (3.23) holds for the computed approximation, one needs the following lemma to derive an estimate which is valid for all decompositions.

Lemma 3.12. *Assume that **(A1)–(A4)** are satisfied. Let $\lambda_1, \lambda_0, C_l, C_6$ be positive constants such that*

$$-\lambda_1 \lambda(s) \le \frac{1}{4}\phi(s) + \lambda_0, \quad \forall\, s \in D(\beta), \tag{3.24}$$

$$-\lambda_1 r + \ln r \le C_l, \quad \forall\, r > 0, \tag{3.25}$$

$$\|v\|_{L^6(\Omega)} \le C_6 \|v\|_V, \quad \forall\, v \in V. \tag{3.26}$$

*For the solution (θ, u, χ, ξ) to the Penrose–Fife system **(PF)** it holds*

$$\frac{1}{2C_6^2}\|u\|^2_{L^2(0,t^*;L^6(\Omega))} + \left\|\sqrt{\eta}\,\frac{\partial\chi}{\partial t}\right\|^2_{L^2(0,t^*;L^2(\Omega))} + \frac{\varepsilon}{2}\|\nabla\chi(t^*)\|^2_{(L^2(\Omega))^N} + \frac{1}{2}\|\phi(\chi(t^*))\|_{L^1(\Omega)}$$
$$\leq \int_\Omega \Big(\lambda_1\big(c_0\theta^0 + \lambda(\chi^0)\big) - c_0\ln\theta^0 + \phi(\chi^0) - \sigma(\chi^0)\Big)\,\mathrm{d}x$$
$$+ \big(c_0 C_l + \lambda_0 + \sigma_0\big)\,|\Omega| + \frac{\varepsilon}{2}\left\|\nabla\chi^0\right\|^2_{(L^2(\Omega))^N} + \frac{1}{\gamma^2}\|\zeta + \gamma\lambda_1\|^2_{L^2(\Gamma\times(0,t^*))}$$
$$+ \lambda_1\|g\|_{L^1(\Omega\times(0,t^*))} + C_*^2\|g\|^2_{L^2(0,t^*;V^*)}, \quad \forall\, t^* \in [0,T]. \tag{3.27}$$

Proof. From **(A2)** and $0 \in D(\beta)$, we get by integration

$$\lambda(s) \geq \frac{1}{2}\lambda_0'' s^2 + \lambda'(0)s + \lambda(0), \quad \forall\, s \in D(\beta).$$

Using now Young's inequality and **(A1)**, we get some positive constants λ_1 and λ_0 such that (3.24) holds. The left–hand side of (3.25) is a continuous differentiable function on $(0,\infty)$, which tends to $-\infty$ at the boundaries of this interval; this yields (3.25). The equivalence of the norms $\|\cdot\|_V$ and $\|\cdot\|_{H^1(\Omega)}$ and the continuous embedding of $H^1(\Omega)$ into $L^6(\Omega)$ gives a constant C_6 such that (3.26) holds.

Now, the main estimate (3.27) will be proved. Let $t^* \in (0,T]$ be given. We multiply (2.1e) by $\lambda_1 - u$ and integrate the resulting equation over $\Omega\times(0,t^*)$. Since (2.1d) yields $u\frac{\partial\theta}{\partial t} = \frac{\partial(\ln\theta)}{\partial t}$, we get by applying (2.1g), (2.1h), (3.1), (3.2), (3.24), (3.25), **(A3)**, and Young's inequality

$$\|u\|^2_{L^2(0,t^*;V)} = \int_\Omega \big(-c_0\lambda_1\theta(t^*) + c_0\ln(\theta(t^*)) + c_0\lambda_1\theta^0 - c_0\ln(\theta^0) - \lambda_1\lambda(\chi(t^*)) + \lambda_1\lambda(\chi^0)\big)\,\mathrm{d}x$$
$$+ \int_0^{t^*}\!\!\int_\Omega \Big(\lambda'(\chi)\frac{\partial\chi}{\partial t}u + g(\lambda_1 - u)\Big)\,\mathrm{d}x\ \mathrm{d}t + \int_0^{t^*}\!\!\int_\Gamma \Big(\zeta(u-\lambda_1) + \gamma\lambda_1 u\Big)\,\mathrm{d}\nu\ \mathrm{d}t$$
$$\leq \int_\Omega \Big(c_0 C_l + c_0\lambda_1\theta^0 - c_0\ln(\theta^0) + \frac{1}{4}\phi(\chi(t^*)) + \lambda_0 + \lambda_1\lambda(\chi^0)\Big)\,\mathrm{d}x$$
$$+ \int_0^{t^*}\!\!\int_\Omega \lambda'(\chi)\frac{\partial\chi}{\partial t}u\,\mathrm{d}x\ \mathrm{d}t + \lambda_1\|g\|_{L^1(\Omega\times(0,t^*))} + C_*^2\|g\|^2_{L^2(0,t^*;V^*)}$$
$$+ \frac{1}{\gamma^2}\|\zeta + \gamma\lambda_1\|^2_{L^2(0,t^*;L^2(\Gamma))} + \frac{1}{2}\|u\|^2_{L^2(0,t^*;V)}. \tag{3.28}$$

Now, (2.1f) is tested by $\frac{\partial\chi}{\partial t}$ and the resulting equation is integrated over $\Omega\times(0,t^*)$. Using that $\eta > 0$ in Ω (see **(A3)**), (2.1g), (2.1h), and **(A2)**, we get

$$\left\| \sqrt{\eta} \frac{\partial \chi}{\partial t} \right\|^2_{L^2(0,t^*;L^2(\Omega))} + \frac{\varepsilon}{2} \|\nabla \chi(t^*)\|^2_{(L^2(\Omega))^N} + \int_0^{t^*} \int_\Omega \xi \frac{\partial \chi}{\partial t} \, \mathrm{d}x \, \mathrm{d}t$$

$$\leq - \int_0^{t^*} \int_\Omega \lambda'(\chi) u \frac{\partial \chi}{\partial t} \, \mathrm{d}x \, \mathrm{d}t + \int_\Omega \Big(\frac{1}{4} \phi(\chi(t^*)) + \sigma_0 - \sigma(\chi^0) \Big) \, \mathrm{d}x + \frac{\varepsilon}{2} \left\| \nabla \chi^0 \right\|^2_{(L^2(\Omega))^N} . \quad (3.29)$$

Since $\xi \in \beta(\chi)$ a.e. in Ω_T (see (2.1d)), by applying **(A1)** and [Bré73, Lemma 3.3] we get

$$\int_0^{t^*} \int_\Omega \xi \frac{\partial \chi}{\partial t} \, \mathrm{d}x \, \mathrm{d}t = \|\phi(\chi(t^*))\|_{L^1(\Omega)} - \left\|\phi(\chi^0)\right\|_{L^1(\Omega)} .$$

Adding now (3.28) to (3.29), and using (3.26) afterwards, we see that (3.27) holds. ☐

Remark 3.13. Using (3.27), for each partition $\mathcal{P}$ of $[0, T]$ we can compute an upper bound for $\|u\|^2_{L^2(0,t_k;L^6(\Omega))}$. This can be used to estimate $\omega_{k,m}$, so that (3.18) reads as a computable a posteriori error estimate. But, this error estimate will be quite pessimistic, as this already holds for the upper bound for $\|u\|^2_{L^2(0,t_k;L^6(\Omega))}$ stated in (3.27). Hence, for practical computations one will to use the a posteriori error estimate derived in Remark 3.11, hoping that (3.23) is satisfied for the considered approximation.

4 Proof of the a posteriori error estimates

4.1 Notations and properties

For preparing the proof of the error estimates, some additional notations are introduced and some useful equalities and inequalities are presented.

In the sequel, we will use, for $p \geq 1$, the notation $\|\cdot\|_p$ for the $L^p(\Omega)$–norm and $\|\cdot\|_{2,N}$ for the $(L^2(\Omega))^N$–norm.

Let $F : V \to V^*$ be the duality mapping:

$$\langle Fw, v \rangle_{V^* \times V} = (w, v)_V , \quad \forall\, w, v \in V. \quad (4.1)$$

We see that V^* is a Hilbert space with the inner product $(\cdot, \cdot)_*$

$$(\psi, \varphi)_* := \left\langle \psi, F^{-1}\varphi \right\rangle_{V^* \times V} = (F^{-1}\psi, F^{-1}\varphi)_V, \quad \forall\, \psi, \varphi \in V^*, \quad (4.2)$$

satisfying

$$\|\psi\|_{V^*} := \sqrt{(\psi, \psi)_*} = \left\|F^{-1}\psi\right\|_V , \quad \forall\, \psi \in V^*. \quad (4.3)$$

By embedding $L^2(\Omega)$ and $L^2(\Gamma)$ into V^*, we get

$$\langle f+\varphi, v\rangle_{V^*\times V} = \int\limits_\Omega f v \,\mathrm{d}x + \int\limits_\Gamma \varphi v \,\mathrm{d}\nu\,, \quad \forall\, v \in V,\ f\in L^2(\Omega),\ \varphi\in L^2(\Gamma). \tag{4.4}$$

Considering the definition (3.4) of l, we see that, for all $m = 1,\dots,M$,

$$\int\limits_{t_{m-1}}^{t_m} l(t)\,\mathrm{d}t = \int\limits_{t_{m-1}}^{t_m} (1-l(t))\,\mathrm{d}t = \frac{h_m}{2}, \quad \int\limits_{t_{m-1}}^{t_m} (l(t))^2\,\mathrm{d}t = \int\limits_{t_{m-1}}^{t_m} (1-l(t))^2\,\mathrm{d}t = \frac{h_m}{3}. \tag{4.5}$$

The following Gronwall–type inequality is a generalization of [NSaV00, Lemma 3.7], where a similar inequality with ψ being a constant is formulated.

Lemma 4.1 (Generalized Gronwall inequality). *Let $a,b,c,d : (0,t^*) \to [0,+\infty]$, with $t^* > 0$, be measurable functions, a^2 also being absolutely continuous on $[0,t^*]$. Let $\psi : (0,t^*) \to \mathbb{R}$ be an integrable function such that the differential inequality holds*

$$\frac{\mathrm{d}a^2(t)}{\mathrm{d}t} + b^2(t) \le c^2(t) + 2d(t)a(t) + 2\psi(t)a^2(t), \quad \text{a.e. in} \quad (0,t^*). \tag{4.6}$$

Then we have:

$$\max\Big\{\max_{t\in[0,t^*]} a(t)\tilde\Psi(t)\,,\ \Big(\int\limits_0^{t^*} b^2(t)\tilde\Psi^2(t)\,\mathrm{d}t\Big)^{1/2}\Big\} \le \Big(a^2(0)\tilde\Psi^2(0) + \int\limits_0^{t^*} c^2(t)\tilde\Psi^2(t)\,\mathrm{d}t\Big)^{1/2} + \int\limits_0^{t^*} d(t)\tilde\Psi(t)\,\mathrm{d}t\,, \tag{4.7}$$

with

$$\tilde\Psi(t) := \exp\Big(\int\limits_t^{t^*}\psi(\tau)\,\mathrm{d}\tau\Big), \quad \forall\, t\in[0,t^*].$$

Proof. Let the functions $v,w : [0,t^*] \to \mathbb{R}$ be defined by

$$v(t) := a^2(t)\tilde\Psi^2(t) + \int\limits_0^t b^2(\tau)\tilde\Psi^2(\tau)\,\mathrm{d}\tau\,,$$

$$w(t) := \Big(\Big(a^2(0)\tilde\Psi^2(0) + \int\limits_0^t c^2(\tau)\tilde\Psi^2(\tau)\,\mathrm{d}\tau\Big)^{1/2} + \int\limits_0^t d(\tau)\tilde\Psi(\tau)\,\mathrm{d}\tau\Big)^2,$$

for all $t\in[0,t^*]$. Following the proof of [NSaV00, Lemma 3.6], one can use (4.6) to show that

$$v'(t) \le c^2(t)\tilde\Psi^2(t) + 2d(t)\tilde\Psi(t)\sqrt{v(t)}, \quad w'(t) \ge c^2(t)\tilde\Psi^2(t) + 2d(t)\tilde\Psi(t)\sqrt{w(t)}, \quad \forall\, t\in[0,t^*].$$

Since $v(0) = w(0) > 0$, a comparison argument for differential inequalities yields $v(t)\le w(t)$ for all $t\in[0,t^*]$. By considering the maximum over $t\in[0,t^*]$ we see that (4.7) holds. $\square$

4.2 Preparation of the estimates

In this subsection it is assumed that **(A1)**–**(A5)** are satisfied. Hence, the time discrete scheme **(D)** has a unique solution. Considering the corresponding piecewise linear and piecewise constant approximations defined in (2.5) and (2.6) and using **(A4)**, equation (2.4) can be rewritten as

$$\widehat{\theta} > 0, \quad \overline{\theta} > 0, \quad \overline{u} > 0, \quad \underline{u} > 0, \quad \overline{u} = \frac{1}{\overline{\theta}}, \quad \text{a.e. in} \quad \Omega_T, \tag{4.8a}$$

$$\overline{\chi}, \underline{\chi} \in D(\beta), \quad \overline{\xi} \in \beta(\overline{\chi}), \quad \text{a.e. in} \quad \Omega_T, \tag{4.8b}$$

$$c_0 \frac{\partial \widehat{\theta}}{\partial t} + \lambda'(\underline{\chi}) \frac{\partial \widehat{\chi}}{\partial t} + \kappa \Delta \overline{u} = \overline{g}, \quad \text{a.e. in} \quad \Omega_T, \tag{4.8c}$$

$$\eta \frac{\partial \widehat{\chi}}{\partial t} - \varepsilon \Delta \overline{\chi} + \overline{\xi} - \sigma''(\underline{\chi}) \overline{\chi} = -\lambda'(\underline{\chi}) \overline{u} - \sigma''(\underline{\chi}) \underline{\chi} + \sigma'(\underline{\chi}), \quad \text{a.e. in} \quad \Omega_T, \tag{4.8d}$$

$$\kappa \frac{\partial \overline{u}}{\partial n} + \gamma \overline{u} = \overline{\zeta}, \quad \frac{\partial \widehat{\chi}}{\partial n} = \frac{\partial \overline{\chi}}{\partial n} = \frac{\partial \underline{\chi}}{\partial n} = 0, \quad \text{a.e. on} \quad \Gamma_T, \tag{4.8e}$$

$$\widehat{\theta}(\cdot, 0) = \theta^0, \quad \widehat{\chi}(\cdot, 0) = \chi^0, \quad \text{a.e. in} \quad \Omega. \tag{4.8f}$$

As abbreviations, we introduce the errors in the approximation of u and χ

$$\overline{e}_u := u - \overline{u}, \quad \overline{e}_\chi := \chi - \overline{\chi}, \quad \widehat{e}_\chi := \chi - \widehat{\chi}, \qquad \text{a.e. in} \quad \Omega_T, \tag{4.9}$$

and the error in the approximation of the internal energy $c_0\theta + \lambda(\chi)$

$$\widehat{e}_I := c_0 \theta + \lambda(\chi) - \big(c_0 \widehat{\theta} + \lambda(\widehat{\chi})\big), \quad \text{a.e. in} \quad \Omega_T. \tag{4.10}$$

Thanks to the initial conditions (2.1h) and (4.8f), we see that

$$\widehat{e}_I(\cdot, 0) = 0, \quad \widehat{e}_\chi(\cdot, 0) = 0, \quad \text{a.e. in} \quad \Omega. \tag{4.11}$$

Also, for $t \in [0, T]$, some combinations of norms of approximation errors will be used:

$$E_0(t) := \|\widehat{e}_I(t)\|_{V^*}^2 + \|\sqrt{\eta}\, \widehat{e}_\chi(t)\|_2^2, \tag{4.12}$$

$$E_1(t) := c_0 l(t) \left\| \frac{\overline{e}_u^2(t)}{u(t)\overline{u}(t)} \right\|_1 + c_0 (1 - l(t)) \left\| \alpha(\overline{u}(t), u(t), \underline{u}(t)) \right\|_1, \tag{4.13}$$

$$E_2(t) := \|\nabla \overline{e}_\chi(t)\|_{2,N}^2 + \|\nabla \widehat{e}_\chi(t)\|_{2,N}^2, \tag{4.14}$$

$$R(t) := -\frac{1}{2} \lambda_0'' \left\| \big(u(t) + \overline{u}(t)\big) \widehat{e}_\chi^2(t) \right\|_1. \tag{4.15}$$

Using the discrete Schwarz inequality, we see that

$$\|\widehat{e}_I(t)\|_{V^*} + \|\sqrt{\eta}\, \widehat{e}_\chi(t)\|_2 \le \sqrt{2} \sqrt{E_0(t)}, \quad \forall\, t \in [0, T]. \tag{4.16}$$

Moreover, for $t \in [0,T]$, it is convenient to define the following quantities, which depend on data and approximate solutions:

$$I_1(t) := \left\| \big(\lambda'(\underline{\chi}(t)) - \lambda'(\widehat{\chi}(t))\big)\frac{\partial \widehat{\chi}}{\partial t}(t) + g(t) - \overline{g}(t) - \big(\zeta(t) - \overline{\zeta}(t)\big) \right\|_{V^*}, \tag{4.17}$$

$$I_2(t) := \frac{1}{\sqrt{\eta_0}} \|\sigma'(\widehat{\chi}(t)) - \sigma'(\underline{\chi}(t)) + \sigma''(\underline{\chi}(t))\big(\underline{\chi}(t) - \overline{\chi}(t)\big)$$
$$+ \big(\lambda'(\underline{\chi}(t)) - \lambda'(\widehat{\chi}(t))\big)\overline{u}(t)\|_2, \tag{4.18}$$

$$I_3(t) := c_0(1 - l(t)) \left\| \frac{(\overline{u}(t) - \underline{u}(t))^2}{\overline{u}(t)\underline{u}(t)} \right\|_1, \tag{4.19}$$

$$I_4(t) := \left\|\overline{\xi}(t)\big(\overline{\chi}(t) - \widehat{\chi}(t)\big) + \phi(\widehat{\chi}(t)) - \phi(\overline{\chi}(t))\right\|_1 + \frac{\varepsilon}{2}\|\nabla(\overline{\chi}(t) - \widehat{\chi}(t))\|_{2,N}^2 . \tag{4.20}$$

In the following, the errors E_0, E_1, E_2 are going to be estimated by $R, I_1, \ldots, I_4$. Afterwards $I_1, \ldots, I_4$ will be estimated by error indicators defined in (3.9) and (3.22). Therein, techniques derived in [NSaV00] are applied and adapted to the specific non–linearities of the Penrose–Fife system.

Lemma 4.2. *We have for a.e. $t \in (0,T)$:*

$$\frac{1}{2}\frac{\mathrm{d}E_0(t)}{\mathrm{d}t} + E_1(t) + \frac{\varepsilon}{2}E_2(t)$$
$$\leq \sqrt{2}\max\big(I_1(t), I_2(t)\big)\sqrt{E_0(t)} + I_3(t) + I_4(t) + \frac{\sigma_1''}{\eta_0}E_0(t) + R(t). \tag{4.21}$$

Proof. By taking the difference of equations (2.1e) and (4.8c) and using notation (4.9) and (4.10), we get

$$\frac{\partial \widehat{e}_I}{\partial t} + \kappa\Delta\overline{e}_u = \lambda'(\underline{\chi})\frac{\partial \widehat{\chi}}{\partial t} - \frac{\partial \lambda(\widehat{\chi})}{\partial t} + g - \overline{g}, \quad \text{a.e. in} \quad \Omega_T.$$

Testing this equation by a function $v \in H^1(\Omega)$, integrating the resulting identity over Ω, using the boundary conditions in (2.1g) and (4.8e), and applying the definitions of the inner product on V in (3.1), we observe that, for a.e. $t \in (0,T)$,

$$\int_\Omega \frac{\partial \widehat{e}_I}{\partial t}(t) v \,\mathrm{d}x - (\overline{e}_u(t), v)_V = -\int_\Gamma \big(\zeta(t) - \overline{\zeta}(t)\big) v \,\mathrm{d}\nu$$
$$+ \int_\Omega \Big(\big(\lambda'(\underline{\chi}(t)) - \lambda'(\widehat{\chi}(t))\big)\frac{\partial \widehat{\chi}}{\partial t}(t) + g(t) - \overline{g}(t)\Big) v \,\mathrm{d}x, \quad \forall\, v \in H^1(\Omega).$$

Combining this with (4.1)–(4.4) and the definition (4.17) of I_1, we get

$$\Big(\frac{\partial \widehat{e}_I}{\partial t}(t), \psi^*\Big)_* - \langle \psi^*, \overline{e}_u(t)\rangle_{V^*\times V} = \int_\Omega \frac{\partial \widehat{e}_I}{\partial t}(t) F^{-1}\psi^* \,\mathrm{d}x - \big(\overline{e}_u(t), F^{-1}\psi^*\big)_V$$
$$\leq I_1(t)\left\|F^{-1}\psi^*\right\|_V = I_1(t)\|\psi^*\|_{V^*}, \quad \forall\, \psi^* \in V^*, \quad \text{for a.e. } t \in (0,T).$$

We select $\psi^* = \widehat{e}_I(t)$ and use (4.10) and (4.4), to arrive at

$$\begin{aligned}&\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\,\|\widehat{e}_I(t)\|_{V^*}^2 - c_0 \int\limits_\Omega \big(\theta(t) - \widehat{\theta}(t)\big)\overline{e}_u(t)\,\mathrm{d}x \\ &\quad\le I_1(t)\,\|\widehat{e}_I(t)\|_{V^*} + \int\limits_\Omega \big(\lambda(\chi(t)) - \lambda(\widehat{\chi}(t))\big)\overline{e}_u(t)\,\mathrm{d}x\,, \quad \text{for a.e. } t \in (0,T).\end{aligned} \tag{4.22}$$

Using (3.5) and the compatibility conditions in (2.1d) and in (4.8a), and recalling the definitions of α, E_1, and I_3, in (3.3), (4.13), and (4.18) respectively, we get

$$\begin{aligned}&- c_0 \int\limits_\Omega \big(\theta(t) - \widehat{\theta}(t)\big)\overline{e}_u(t)\,\mathrm{d}x \;= c_0 l(t)\left\|\frac{(u(t)-\overline{u}(t))^2}{u(t)\overline{u}(t)}\right\|_1 \\ &\quad + c_0(1-l(t))\int\limits_\Omega \Big(\alpha(\overline{u}(t),u(t),\underline{u}(t)) - \big(\overline{u}(t)-\underline{u}(t)\big)\Big(\frac{1}{\underline{u}(t)} - \frac{1}{\overline{u}(t)}\Big)\Big)\,\mathrm{d}x \;= E_1(t) - I_3(t).\end{aligned}$$

We use this equation to rewrite (4.22) as

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\,\|\widehat{e}_I(t)\|_{V^*}^2 + E_1(t) \le I_1(t)\,\|\widehat{e}_I(t)\|_{V^*} + \int\limits_\Omega \big(\lambda(\chi(t)) - \lambda(\widehat{\chi}(t))\big)\overline{e}_u(t)\,\mathrm{d}x \,+ I_3(t). \tag{4.23}$$

Now we take the difference of the equations (2.1f) and (4.8d) and test by $\widehat{e}_\chi(t)$. Applying the boundary conditions (2.1g) and (4.8e), the definition (4.18) of I_2, and Young's inequality, we obtain, for a.e. $t \in (0,T)$,

$$\begin{aligned}&\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\,\|\sqrt{\eta}\,\widehat{e}_\chi(t)\|_2^2 + \varepsilon\int\limits_\Omega \nabla\overline{e}_\chi(t)\cdot\nabla\widehat{e}_\chi(t)\,\mathrm{d}x \\ &\quad= \int\limits_\Omega \Big(\lambda'(\underline{\chi}(t))\overline{u}(t) - \lambda'(\chi(t))u(t) + \overline{\xi}(t) - \xi(t) \\ &\qquad + \sigma'(\chi(t)) - \sigma'(\underline{\chi}(t)) - \sigma''(\underline{\chi}(t))\big(\overline{\chi}(t) - \underline{\chi}(t)\big)\Big)\widehat{e}_\chi(t)\,\mathrm{d}x \\ &\quad\le \int\limits_\Omega \big(\overline{\xi}(t) - \xi(t)\big)\widehat{e}_\chi(t)\,\mathrm{d}x \,+ \sqrt{\eta_0}I_2(t)\,\|\widehat{e}_\chi(t)\|_2 \\ &\qquad + \int\limits_\Omega \Big(\lambda'(\widehat{\chi}(t))\overline{u}(t) - \lambda'(\chi(t))u(t) + \sigma'(\chi(t)) - \sigma'(\widehat{\chi}(t))\Big)\widehat{e}_\chi(t)\,\mathrm{d}x\,.\end{aligned} \tag{4.24}$$

Using (4.9), (4.14), and the equality $2(a-b)(a-c) = (a-b)^2 + (a-c)^2 - (b-c)^2$ (which follows directly from the second binomial formula), we see that

$$\int\limits_\Omega \nabla\overline{e}_\chi(t)\cdot\nabla\widehat{e}_\chi(t)\,\mathrm{d}x \;= \frac{1}{2}E_2(t) - \frac{1}{2}\,\|\nabla\overline{\chi}(t) - \nabla\widehat{\chi}(t)\|_{2,N}^2\,. \tag{4.25}$$

We invoke the compatibility conditions in (2.1d) and in (4.8b), and use **(A1)**, to show that

$$\begin{aligned}(\overline{\xi}-\xi)\widehat{e}_\chi &= \xi(\widehat{\chi}-\chi)+\overline{\xi}\big(\chi-\overline{\chi}+(\overline{\chi}-\widehat{\chi})\big)\\ &\le \phi(\widehat{\chi})-\phi(\chi)+\phi(\chi)-\phi(\overline{\chi})+\overline{\xi}(\overline{\chi}-\widehat{\chi})\\ &= \big|\overline{\xi}(\overline{\chi}-\widehat{\chi})+\phi(\widehat{\chi})-\phi(\overline{\chi})\big|, \quad \text{a.e. in} \quad \Omega_T. \end{aligned} \tag{4.26}$$

Combining (4.24)–(4.26), **(A2)**, property $\eta \ge \eta_0$ in **(A3)**, and (4.20), we get

$$\begin{aligned}&\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\,\|\sqrt{\eta}\,\widehat{e}_\chi(t)\|_2^2+\frac{\varepsilon}{2}E_2(t)\le I_2(t)\,\|\sqrt{\eta}\,\widehat{e}_\chi(t)\|_2+I_4(t)\\ &\quad -\int_\Omega \big(\lambda'(\chi(t))u(t)-\lambda'(\widehat{\chi}(t))\overline{u}(t)\big)\widehat{e}_\chi(t)\,\mathrm{d}x+\frac{\sigma_1''}{\eta_0}\,\|\sqrt{\eta}\,\widehat{e}_\chi(t)\|_2^2, \quad \text{for a.e. } t\in(0,T).\end{aligned}$$

Adding this inequality to (4.23), we arrive at

$$\begin{aligned}&\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\,\|\widehat{e}_I(t)\|_{V^*}^2+E_1(t)+\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\,\|\sqrt{\eta}\,\widehat{e}_\chi(t)\|_2^2+\frac{\varepsilon}{2}E_2(t)\\ &\quad\le I_1(t)\,\|\widehat{e}_I(t)\|_{V^*}+I_2(t)\,\|\sqrt{\eta}\,\widehat{e}_\chi(t)\|_2+\frac{\sigma_1''}{\eta_0}\,\|\sqrt{\eta}\,\widehat{e}_\chi(t)\|_2^2+I_3(t)+I_4(t)\\ &\qquad+\int_\Omega\Big(\big(\lambda(\chi(t))-\lambda(\widehat{\chi}(t))\big)\overline{e}_u(t)-\big(\lambda'(\chi(t))u(t)-\lambda'(\widehat{\chi}(t))\overline{u}(t)\big)\widehat{e}_\chi(t)\Big)\,\mathrm{d}x\,,\end{aligned} \tag{4.27}$$

for a.e. $t\in(0,T)$. Applying Taylor's formula and **(A2)**, we see that a.e. in Ω_T it holds

$$\begin{aligned}&\big(\lambda(\chi)-\lambda(\widehat{\chi})\big)\overline{e}_u-\big(\lambda'(\chi)u-\lambda'(\widehat{\chi})\overline{u}\big)\widehat{e}_\chi\\ &\quad= u\big(\lambda(\chi)+\lambda'(\chi)(\widehat{\chi}-\chi)-\lambda(\widehat{\chi})\big)+\overline{u}\big(\lambda(\widehat{\chi})+\lambda'(\widehat{\chi})(\chi-\widehat{\chi})-\lambda(\chi)\big)\\ &\quad\le -\frac{1}{2}\lambda_0''(u+\overline{u})(\chi-\widehat{\chi})^2.\end{aligned}$$

Inserting this inequality in (4.27) and using the definition (4.15) of $R(t)$, we conclude that

$$\begin{aligned}&\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\big(\,\|\widehat{e}_I(t)\|_{V^*}^2+\|\sqrt{\eta}\,\widehat{e}_\chi(t)\|_2^2\,\big)+E_1(t)+\frac{\varepsilon}{2}E_2(t)\\ &\quad\le \max\big(I_1(t),I_2(t)\big)\big(\,\|\widehat{e}_I(t)\|_{V^*}+\|\sqrt{\eta}\,\widehat{e}_\chi(t)\|_2\,\big)+\frac{\sigma_1''}{\eta_0}\,\|\sqrt{\eta}\,\widehat{e}_\chi(t)\|_2^2+I_3(t)+I_4(t)+R(t),\end{aligned}$$

for a.e. $t\in(0,T)$. Recalling (4.12) and (4.16), we conclude that (4.21) is proved. □

Now we bound $I_1(t),\dots,I_4(t)$ in terms of the estimators $\mathcal{E}_{1,m},\mathcal{E}_{4,m},\mathcal{E}_{5,m},\mathcal{E}_{6,m}$.

Lemma 4.3. *For $m=1,\dots,M$ it holds*

$$\int_{t_{m-1}}^{t_m}\big(I_1(t)+I_2(t)\big)\,\mathrm{d}t\;\le\frac{h_m}{2}(\mathcal{E}_{4,m}+\mathcal{E}_{5,m}+\mathcal{E}_{6,m}). \tag{4.28}$$

Proof. Let $1 \le m \le M$ be arbitrary. Consider first term I_1 defined in (4.17). Using (2.5), (2.6), (3.2), and (3.6), we obtain that, for $t \in (t_{m-1}, t_m]$,

$$I_1(t) \le \frac{C_*}{h_m} \left\| \left(\lambda'(\widehat{\chi}(t)) - \lambda'(\chi_{m-1})\right)\delta\chi_m \right\|_{L^2(\Omega)} + \|g(t) - g_m\|_{V^*} + \frac{1}{\gamma}\|\zeta(t) - \zeta_m\|_{L^2(\Gamma)}. \quad (4.29)$$

Applying Taylor's formula, by virtue of **(A2)**, (3.5), and (3.6), we get, a.e. in $\Omega \times (t_{m-1}, t_m]$,

$$|\lambda'(\widehat{\chi}) - \lambda'(\chi_{m-1})| = |\lambda'(l\chi_m + (1-l)\chi_{m-1}) - \lambda'(\chi_{m-1})| \le \max\left(|\lambda_0''|, \lambda_1''\right) l\, |\delta\chi_m|. \quad (4.30)$$

Hence, taking (4.29), (3.9d), (4.5), and (3.22a) into account, we deduce that

$$\int_{t_{m-1}}^{t_m} I_1(t)\,\mathrm{d}t \le \frac{C_*}{h_m}\max\left(|\lambda_0''|, \lambda_1''\right)\int_{t_{m-1}}^{t_m} l(t)\left\|(\delta\chi_m)^2\right\|_2 \mathrm{d}t + \frac{h_m}{2}\mathcal{E}_{4,m} = \frac{h_m}{2}(\mathcal{E}_{4,m} + \mathcal{E}_{5,m}). \quad (4.31)$$

Now we consider term I_2 defined in (4.18). Using (2.5), (2.6), and (3.5), we obtain that, for $t \in (t_{m-1}, t_m]$,

$$\begin{aligned} I_2(t) \le \frac{1}{\sqrt{\eta_0}}\Big(&\|\sigma'(l(t)\chi_m + (1-l(t))\chi_{m-1}) - \sigma'(\chi_{m-1}) + \sigma''(\chi_{m-1})(\chi_{m-1} - \chi_m)\|_2 \\ &+ \left\|\left(\lambda'(\chi_{m-1}) - \lambda'(\widehat{\chi}(t))\right)u_m\right\|_2\Big). \end{aligned} \quad (4.32)$$

Applying Taylor's formula and using **(A2)**, (3.5), and (3.6), we can show that, a.e. in $\Omega \times (t_{m-1}, t_m]$,

$$\begin{aligned} &|\sigma'(l\chi_m + (1-l)\chi_{m-1}) - \sigma'(\chi_{m-1}) + \sigma''(\chi_{m-1})(\chi_{m-1} - \chi_m)| \\ &\quad \le \sigma_1''(1-l)\,|\delta\chi_m| + \frac{1}{2}\sigma_1''' l^2 (\delta\chi_m)^2. \end{aligned}$$

Thanks to this estimate, (4.30), (4.5), and (3.22b), from (4.32) we see that

$$\begin{aligned} \int_{t_{m-1}}^{t_m} I_2(t)\,\mathrm{d}t \le \frac{1}{\sqrt{\eta_0}}\int_{t_{m-1}}^{t_m} \Big(&(1 - l(t))\sigma_1''\,\|\delta\chi_m\|_2 + \frac{1}{2}l^2(t)\sigma_1'''\,\|\delta\chi_m\|_4^2 \\ &+ l(t)\max\left(|\lambda_0''|, \lambda_1''\right)\|u_m\delta\chi_m\|_2\Big)\,\mathrm{d}t = \frac{h_m}{2}\mathcal{E}_{6,m}. \end{aligned}$$

Adding this estimate to (4.31), we conclude that (4.28) holds. □

Lemma 4.4. *For $m = 1, \ldots, M$ it holds*

$$\int_{t_{m-1}}^{t_m} \left(I_3(t) + I_4(t)\right)\mathrm{d}t \le \frac{h_m}{4}\mathcal{E}_{1,m}. \quad (4.33)$$

Proof. Let $1 \le m \le M$ be arbitrary. Consider first term I_4 defined in (4.20). Using formula (3.5) for $\widehat{\chi}$, (3.6), the compatibility condition (2.4c), and the convexity of ϕ in **(A1)**, we conclude that, a.e. in $\Omega \times (t_{m-1}, t_m]$,

$$\begin{aligned}&\left|\overline{\xi}(\overline{\chi} - \widehat{\chi}) + \phi(\widehat{\chi}) - \phi(\overline{\chi})\right| \\ &\quad \le \xi_m\big(\chi_m - (l\chi_m + (1-l)\chi_{m-1})\big) + \big(l\phi(\chi_m) + (1-l)\phi(\chi_{m-1})\big) - \phi(\chi_m) \\ &\quad = (1-l)\big(\xi_m \delta\chi_m - \delta\phi_m\big) = \big|(1-l)\big(\xi_m\delta\chi_m - \delta\phi_m\big)\big| .\end{aligned}$$

Therefore, on using again (3.5) and (3.6) in conjunction with (4.5), we see from (4.20) that

$$\begin{aligned}\int_{t_{m-1}}^{t_m} I_4(t)\,\mathrm{d}t &\le \int_{t_{m-1}}^{t_m} \Big((1-l(t))\,\|\xi_m\delta\chi_m - \delta\phi_m\|_1 + \frac{\varepsilon}{2}(1-l(t))^2\,\|\nabla\delta\chi_m\|_{2,N}^2 \Big)\,\mathrm{d}t \\ &= \frac{h_m}{2}\,\|\xi_m\delta\chi_m - \delta\phi_m\|_1 + \frac{\varepsilon h_m}{6}\,\|\nabla\delta\chi_m\|_{2,N}^2 . \end{aligned} \tag{4.34}$$

Now we consider term I_3 defined in (4.19). In view of (2.6), (3.6), and (4.5), we can easily get

$$\int_{t_{m-1}}^{t_m} I_3(t)\,\mathrm{d}t = c_0 \int_{t_{m-1}}^{t_m} (1-l(t)) \left\| \frac{(\delta u_m)^2}{u_m u_{m-1}} \right\|_1 \mathrm{d}t = \frac{c_0 h_m}{2} \left\| \frac{(\delta u_m)^2}{u_m u_{m-1}} \right\|_1 .$$

Adding this to (4.34), and recalling the definition (3.9a) of $\mathcal{E}_{1,m}$, we see that (4.33) holds. □

4.3 Proof of Theorem 3.5 and Corollary 3.1

In this subsection, Theorem 3.5 and Corollary 3.1 will be proved. It is assumed that **(A1)**–**(A5)** and $\lambda_0'' \ge 0$ are satisfied.

Let $1 \le k \le M$ be given. Because of (4.15), (2.1d), (4.8a), **(A3)**, and (4.12), we see that

$$R(t) \le -\frac{1}{2}\lambda_0'' \min_{x\in\overline{\Omega}} \overline{u}(x,t)\,\|\widehat{e}_\chi(t)\|_2^2 \le -\frac{\lambda_0''}{2\eta_1} \min_{x\in\overline{\Omega}} \overline{u}(x,t) E_0(t), \quad \forall\, t \in [0,T].$$

Defining

$$\psi(t) := \frac{\sigma_1''}{\eta_0} - \frac{\lambda_0''}{2\eta_1} \min_{x\in\overline{\Omega}} \overline{u}(x,t), \quad \forall\, t \in [0,T],$$

we get therefore from Lemma 4.2 that, for a.e. $t \in (0,T)$,

$$\frac{\mathrm{d}E_0(t)}{\mathrm{d}t} + 2E_1(t) + \varepsilon E_2(t) \le 2\sqrt{2}\big(I_1(t) + I_2(t)\big)\sqrt{E_0(t)} + 2\big(I_3(t) + I_4(t)\big) + 2\psi(t)E_0(t). \tag{4.35}$$

Since $\overline{u}$ is piecewise constant, for all $m = 1, \ldots, k$ and all $t \in (t_{m-1}, t_m]$, we have

$$\int_t^{t_k} \psi(\tau)\,\mathrm{d}\tau = \int_t^{t_k} \frac{\sigma_1''}{\eta_0}\,\mathrm{d}t - \frac{\lambda_0''}{2\eta_1}\Big(\int_t^{t_m} \min_{x\in\overline{\Omega}} u_m(x)\,\mathrm{d}t + \sum_{i=m+1}^{k} \int_{t_{i-1}}^{t_i} \min_{x\in\overline{\Omega}} u_i(x)\,\mathrm{d}t \Big),$$

whence, from the definition (3.15) of Ψ_k,

$$\exp\Big(\int_t^{t_k}\psi(\tau)\,\mathrm{d}\tau\Big) = \Psi_k(t), \quad \forall\, t\in[0,t_k].$$

Since $E_0(0) = 0$ because of (4.11) and (4.12), applying to (4.35) the generalized Gronwall inequality (4.7) for $t^* := t_k$, we get therefore

$$\begin{aligned}\mathrm{I} &:= \max\Big\{\max_{t\in[0,t_k]}\big(\sqrt{E_0(t)}\Psi_k(t)\big),\ \Big(\int_0^{t_k}\big(2E_1(t)+\varepsilon E_2(t)\big)\Psi_k^2(t)\,\mathrm{d}t\Big)^{1/2}\Big\}\\ &\le \Big(\int_0^{t_k} 2\big(I_3(t)+I_4(t)\big)\Psi_k^2(t)\,\mathrm{d}t\Big)^{1/2} + \int_0^{t_k}\sqrt{2}\big(I_1(t)+I_2(t)\big)\Psi_k(t)\,\mathrm{d}t \ =: \mathrm{II}. \qquad (4.36)\end{aligned}$$

Using now (4.16), (4.13), (4.14), and the discrete Schwarz inequality, we easily obtain

$$\begin{aligned}\mathrm{I} \ge \frac{1}{\sqrt{2}}\max\Big\{ &\|\Psi_k\widehat{e}_I\|_{C([0,t_k],V^*)}\ ,\ \|\Psi_k\sqrt{\eta}\,\widehat{e}_\chi\|_{C([0,t_k];L^2(\Omega))}\ ,\\ &\Big(2c_0\int_0^{t_k}\Big(l(t)\Big\|\frac{\overline{e}_u^2(t)}{u(t)\overline{u}(t)}\Big\|_1 + (1-l(t))\,\|\alpha(\overline{u}(t),u(t),\underline{u}(t))\|_1\Big)\Psi_k^2(t)\,\mathrm{d}t\Big)^{1/2}\\ &+\Big(\varepsilon\int_0^{t_k}\big(\|\nabla\overline{e}_\chi(t)\|_{2,N}^2 + \|\nabla\widehat{e}_\chi(t)\|_{2,N}^2\big)\Psi_k^2(t)\,\mathrm{d}t\Big)^{1/2}\Big\}. \qquad (4.37)\end{aligned}$$

Applying the upper bound in (3.16), Lemma 4.3, and Lemma 4.4, we deduce that

$$\begin{aligned}\mathrm{II} &\le \Big(2\sum_{m=1}^{k}\max(\psi_{k,m-1}^2,\psi_{k,m}^2)\int_{t_{m-1}}^{t_m}\big(I_3(t)+I_4(t)\big)\,\mathrm{d}t\Big)^{1/2}\\ &\quad+\sqrt{2}\sum_{m=1}^{k}\max(\psi_{k,m-1},\psi_{k,m})\int_{t_{m-1}}^{t_m}\big(I_1(t)+I_2(t)\big)\,\mathrm{d}t\\ &\le \frac{1}{\sqrt{2}}\Big(\sum_{m=1}^{k}h_m\mathcal{E}_{1,m}\max(\psi_{k,m-1}^2,\psi_{k,m}^2)\Big)^{1/2}\\ &\quad+\frac{1}{\sqrt{2}}\sum_{m=1}^{k}h_m\big(\mathcal{E}_{4,m}+\mathcal{E}_{5,m}+\mathcal{E}_{6,m}\big)\max(\psi_{k,m-1},\psi_{k,m}). \qquad (4.38)\end{aligned}$$

Since **(A2)** and $\lambda_0'' \ge 0$ yields that $|\lambda_0''| \le \lambda_1''$, we conclude from Remark 3.9 that $\mathcal{E}_{2,m} = \mathcal{E}_{5,m}$ and $\mathcal{E}_{3,m} = \mathcal{E}_{6,m}$. Combining this with inequalities (4.38), (4.37), and (4.36) and definitions (4.9) and (4.10) leads to (3.14). This finishes the proof of Theorem 3.5. Moreover, taking also (3.16) into account we get (3.7), so that Corollary 3.1 is proved too. □

4.4 Proof of Theorem 3.8

We conclude the paper with the proof of Theorem 3.8. It is assumed that **(A1)**–**(A5)** are satisfied. Since convexity of λ, i.e. $\lambda''(s) \geq \lambda''_0 \geq 0$ in **(A2)**, was essential in treating term $R(t)$ in the proof of Theorem 3.5, we have to argue differently to cover also the general case, where λ''_0 may be negative. Applying the Gagliardo–Nirenberg inequality (see, e.g., [Zhe95, Theorem 1.1.4]), there are two positive constants C_1, C_2 such that

$$\|v\|_3 \leq C_1 \|\nabla v\|_{2,N}^{1/2} \|v\|_2^{1/2} + C_2 \|v\|_2 , \quad \forall\, v \in H^1(\Omega).$$

Thanks to Young's inequality, there is a then constant C_ε such that (3.17) holds. Using this, together with the generalized Hölder's inequality and Young's inequality, from (4.15) we get

$$\begin{aligned} R(t) &\leq \frac{1}{2} |\lambda''_0| \, \|u(t) + \overline{u}(t)\|_{L^6(\Omega)} \, \|\widehat{e}_\chi(t)\|_{L^2(\Omega)} \big(\sqrt{\varepsilon}\, \|\nabla \widehat{e}_\chi(t)\|_{2,N} + C_\varepsilon \, \|\widehat{e}_\chi(t)\|_2 \big) \\ &\leq \frac{\varepsilon}{4} \|\nabla \widehat{e}_\chi(t)\|_{2,N}^2 + \frac{1}{4} |\lambda''_0|^2 \, \|u(t) + \overline{u}(t)\|_{L^6(\Omega)}^2 \, \|\widehat{e}_\chi(t)\|_{L^2(\Omega)}^2 \\ &\quad + \frac{1}{2} |\lambda''_0| \, C_\varepsilon \, \|u(t) + \overline{u}(t)\|_{L^6(\Omega)} \, \|\widehat{e}_\chi(t)\|_{L^2(\Omega)}^2 , \quad \forall\, t \in [0,T]. \end{aligned} \tag{4.39}$$

Setting

$$v(t) := \frac{1}{4\eta_0} |\lambda''_0| \, \|u(t) + \overline{u}(t)\|_{L^6(\Omega)} \big(2C_\varepsilon + |\lambda''_0| \, \|u(t) + \overline{u}(t)\|_{L^6(\Omega)} \big) + \frac{\sigma''_1}{\eta_0}, \tag{4.40}$$

and using (4.39), (4.14), property $\eta \geq \eta_0$ in **(A3)**, and (4.12), from Lemma 4.2 we deduce

$$\frac{\mathrm{d}E_0(t)}{\mathrm{d}t} + 2E_1(t) + \varepsilon \tilde{E}_2(t) \leq 2\sqrt{2}\big(I_1(t) + I_2(t)\big)\sqrt{E_0(t)} + 2\big(I_3(t) + I_4(t)\big) + 2v(t)E_0(t), \tag{4.41}$$

for a.e. $t \in (0,T)$, where

$$\tilde{E}_2(t) := E_2(t) - \frac{1}{2} \|\nabla \widehat{e}_\chi(t)\|_{2,N}^2 = \|\nabla \overline{e}_\chi(t)\|_{2,N}^2 + \frac{1}{2} \|\nabla \widehat{e}_\chi(t)\|_{2,N}^2 .$$

Applying to (4.41) the generalized Gronwall inequality (4.7) for $t^* := t_k$, and taking into account that $E_0(0) = 0$ because of (4.11) and (4.12), we see that

$$\begin{aligned} \mathrm{I} &:= \max\Big\{ \max_{t \in [0,t_k]} \big(\sqrt{E_0(t)}\, \tilde{\Upsilon}_k(t)\big), \Big(\int_0^{t_k} \big(2E_1(t) + \varepsilon \tilde{E}_2(t)\big) \tilde{\Upsilon}_k^2(t)\, \mathrm{d}t \Big)^{1/2} \Big\} \\ &\leq \Big(\int_0^{t_k} 2\big(I_3(t) + I_4(t)\big) \tilde{\Upsilon}_k^2(t)\, \mathrm{d}t \Big)^{1/2} + \int_0^{t_k} \sqrt{2}\big(I_1(t) + I_2(t)\big) \tilde{\Upsilon}_k(t)\, \mathrm{d}t =: \mathrm{II}, \end{aligned} \tag{4.42}$$

where

$$\tilde{\Upsilon}_k(t) := \exp\Big(\int\limits_t^{t_k} v(\tau)\,\mathrm{d}\tau \Big). \tag{4.43}$$

Now we argue as in the proof of Theorem 3.5 to estimate the two terms I and II in (4.42). First, in view of the positivity of both u and $\overline{u}$, we note that $\tilde{\Upsilon}_k(t)$ can be bounded from below by $\Upsilon_k(t)$ defined in (3.19). From (4.40) and (4.43) we have in fact, for all $t \in [0,T]$,

$$\tilde{\Upsilon}_k(t) \geq \exp\Big(\frac{1}{4\eta_0} |\lambda_0''| \int\limits_t^{t_k} \|\overline{u}(\tau)\|_{L^6(\Omega)} \big(2C_\varepsilon + |\lambda_0''|\, \|\overline{u}(\tau)\|_{L^6(\Omega)}\big)\,\mathrm{d}\tau + \frac{\sigma_1''}{\eta_0}(t_k - t)\Big) = \Upsilon_k(t).$$

Therefore, arguing as in the proof of Theorem 3.5, we see that term $\sqrt{2}\,\mathrm{I}$ is bigger than the left hand side of the desired estimate (3.18). For term II, we argue again as in the proof of Theorem 3.5, that is we apply Lemma 4.3 and Lemma 4.4, to arrive at

$$\sqrt{2}\mathrm{II} \leq \Big(\sum_{m=1}^{k} h_m \mathcal{E}_{1,m} \|\tilde{\Upsilon}_k\|^2_{L^\infty(t_{m-1},t_m)} \Big)^{1/2} + \sum_{m=1}^{k} h_m \big(\mathcal{E}_{4,m} + \mathcal{E}_{5,m} + \mathcal{E}_{6,m}\big) \|\tilde{\Upsilon}_k\|_{L^\infty(t_{m-1},t_m)}.$$

Therefore, to conclude the proof of (3.18), it remains to estimate $\|\tilde{\Upsilon}_k\|_{L^\infty(t_{m-1},t_m)}$ from above. From (4.40) and Young's inequality, we see that, for $t \in (t_{m-1}, t_m]$, $m = 1, \ldots, k$,

$$\int\limits_t^{t_k} v(\tau)\,\mathrm{d}\tau \leq \frac{\sigma_1''}{\eta_0}(t_k - t_{m-1}) + \frac{1}{4\eta_0} |\lambda_0''| \int\limits_{t_{m-1}}^{t_k} \Big(2C_\varepsilon \big(\|\overline{u}(\tau)\|_{L^6(\Omega)} + \|u(\tau)\|_{L^6(\Omega)} \big)$$
$$+ |\lambda_0''| \big(2\, \|\overline{u}(\tau)\|^2_{L^6(\Omega)} + 2\, \|u(\tau)\|^2_{L^6(\Omega)} \big) \Big)\,\mathrm{d}\tau\,,$$

whence, in view of (4.43), (3.20), and (3.21),

$$\tilde{\Upsilon}_k(t) \leq v_{k,m}\omega_{k,m} \exp\Big(\frac{\sigma_1''}{\eta_0}(t_k - t_{m-1}) \Big), \quad \forall\, t \in (t_{m-1}, t_m],\ m = 1, \ldots, k. \quad \square$$

Acknowledgements

Olaf Klein would like to thank Prof. Giuseppe Savaré for fruitful discussions.

References

[Bré73] H. Brézis. *Opérateurs maximaux monotones et semi-groupes de contractions dans les espaces de Hilbert*, volume 5 of *North-Holland Mathematics Studies*. North-Holland Publishing Co., Amsterdam, 1973. Notas de Matemática (50).

[CL98] P. Colli and Ph. Laurençot. Weak solutions to the Penrose–Fife phase field model for a class of admissible heat flux laws. *Phys. D*, 111:311–334, 1998.

[CLS99] P. Colli, Ph. Laurençot, and J. Sprekels. Global solution to the Penrose-Fife phase field model with special heat flux laws. In *Variations of domain and free-boundary problems in solid mechanics (Paris, 1997)*, pages 181–188. Kluwer Acad. Publ., Dordrecht, 1999.

[CNS00] Z. Chen, R.H. Nochetto, and A. Schmidt. Error control and adaptivity for a phase relaxation model. *M2AN Math. Model. Numer. Anal.*, 34:775–797, 2000.

[CS98] P. Colli and J. Sprekels. Weak solution to some Penrose–Fife phase–field systems with temperature–dependent memory. *J. Differential Equations*, 142(1):54–77, 1998.

[DK97] A. Damlamian and N. Kenmochi. Evolution equations associated with non-isothermal phase transitions. In *Functional analysis and global analysis (Quezon City, 1996)*, pages 62–77. Springer, Singapore, 1997.

[HLS96] W. Horn, Ph. Laurençot, and J. Sprekels. Global solutions to a Penrose–Fife phase–field model under flux boundary conditions for the inverse temperature. *Math. Methods Appl. Sci.*, 19:1053–1072, 1996.

[Hor93] W. Horn. A numerical scheme for the one–dimensional Penrose–Fife model for phase transitions. *Adv. Math. Sci. Appl.*, 2(2):457–483, 1993.

[HSZ96] W. Horn, J. Sprekels, and S. Zheng. Global existence of smooth solutions to the Penrose–Fife model for Ising ferromagnets. *Adv. Math. Sci. Appl.*, 6:227–241, 1996.

[KK99] N. Kenmochi and M. Kubo. Weak solutions of nonlinear systems for non–isothermal phase transitions. *Adv. Math. Sci. Appl.*, 9(1):499–521, 1999.

[Kle] O. Klein. Existence and approximation of solutions to an anisotropic phase field system of penrose–fife type. *Interfaces Free Bound.* to appear.

[Kle97] O. Klein. A semidiscrete scheme for a Penrose–Fife system and some Stefan problems in $\mathbb{R}^3$. *Adv. Math. Sci. Appl.*, 7(1):491–523, 1997.

[Kle99] O. Klein. A class of time discrete schemes for a phase–field system of Penrose–Fife type. *M2AN Math. Model. Numer. Anal.*, 33(6):1361–1292, 1999.

[KN94] N. Kenmochi and M. Niezgódka. Systems of nonlinear parabolic equations for phase change problems. *Adv. Math. Sci. Appl.*, 3:89–185, 1993/94.

[Lau93] Ph. Laurençot. *Etude de quelques Problèmes aux Dérivées Partielles non Linéaires*. PhD thesis, Université de Franche–Comté, 1993.

[Lau95] Ph. Laurençot. Weak solutions to a Penrose–Fife model for phase transitions. *Adv. Math. Sci. Appl.*, 5(1):117–138, 1995.

[Lau98] Ph. Laurençot. Weak solutions to a Penrose–Fife model with Fourier law for the temperature. *J. Math. Anal. Appl.*, 219:331–343, 1998.

[NSaV00] R.H. Nochetto, G. Savaré, and C. Verdi. A posteriori error estimates for variable time-step discretizations of nonlinear evolution equations. *Comm. Pure Appl. Math.*, 53(5):525–589, 2000.

[NScV00] R.H. Nochetto, A. Schmidt, and C. Verdi. A posteriori error estimation and adaptivity for degenerate parabolic problems. *Math. Comp.*, 69(229):1–24, 2000.

[PF90] O. Penrose and P.C. Fife. Thermodynamically consistent models of phase–field type for the kinetics of phase transitions. *Phys. D*, 43:44–62, 1990.

[Sim87] J. Simon. Compact sets in the space $L^p(0,T;B)$. *Ann. Mat. Pura Appl. (4)*, 146:65–96, 1987.

[SZ93] J. Sprekels and S. Zheng. Global smooth solutions to a thermodynamically consistent model of phase–field type in higher space dimensions. *J. Math. Anal. Appl.*, 176(1):200–223, 1993.

[Zhe95] S. Zheng. *Nonlinear parabolic equations and hyperbolic–parabolic coupled systems*, volume 76 of *Pitman Monographs and Surveys in Pure and Applied Mathematics*. Longman, 1995.