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A SPLITTING SCHEME FOR THE NUMERICAL SOLUTION OF THE KOBAYASHI-WARREN-CARTER SYSTEM

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ABSTRACT. We consider a splitting method for the numerical solution of the regularized Kobayashi-Warren-Carter (KWC) system which describes the growth of single crystal particles of different orientations in two spatial dimensions. The KWC model is a system of two nonlinear parabolic PDEs representing gradient flows associated with a free energy in two variables. Based on an implicit time discretization by the backward Euler method, we suggest a splitting method and prove the existence as well as the energy stability of a solution. The discretization in space is taken care of by Lagrangian finite elements with respect to a geometrically conforming, shape regular, simplicial triangulation of the computational domain and requires the successive solution of two individual discrete elliptic problems. Viewing the time as a parameter, the fully discrete equations represent a parameter dependent nonlinear system which is solved by a predictor corrector continuation strategy with an adaptive choice of the time step size. Numerical results illustrate the performance of the splitting method.

1. INTRODUCTION

The Kobayashi-Warren-Carter (KWC) system is an orientation field based multiphase field model describing the growth of single crystal particles of different orientations in two spatial dimensions. It has been originally suggested in [19, 31] (cf. also [25, 32]) and further studied in [14, 15, 16]. We refer to the monograph [25] for further references. The KWC model is a system of two nonlinear parabolic PDEs representing gradient flows associated with a free energy in two variables, namely the orientation angle and the orientation order (local degree of crystallinity). In particular, the equation with regard to the orientation angle is a second order total variation flow. A mathematical analysis of the KWC system has been provided in [11, 18, 21, 22] mainly focusing on results concerning the existence of a solution. Splitting methods for the numerical solution of PDEs go back to the seminal work [24] and have been further studied in [28] (cf. also the monographs [13, 30] and the review article [20] as well as the references therein).

In this paper, we consider a standard regularization of the total variation flow and focus on an approximation of the thus regularized KWC system by a splitting scheme based on an implicit discretization in time by the backward Euler method.

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The splitting allows to treat the problems in the orientation angle and the orientation order independently at each time step. We prove the existence and energy stability of a solution. For discretization in space we use Lagrangian finite elements with respect to a geometrically conforming, shape regular, simplicial triangulation of the computational domain. Considering the time as a parameter, the fully discrete nonlinear equations represent a parameter dependent nonlinear system which is solved by a predictor-corrector continuation strategy (cf. [6, 17]). This strategy consists of constant continuation as a predictor and Newton's method as a corrector and features an adaptive choice of the time step. Numerical results are provided that illustrate the performance of the splitting scheme.

In this paper, we use standard notation from Lebesgue and Sobolev space theory (cf., e.g., [29]) and the theory of functions of bounded variation (cf., e.g., [1, 7, 12]) and functions of weighted bounded variation (cf. [2]). In particular, for a bounded domain $\Omega \subset \mathbb{R}^d, d \in \mathbb{N}$, we refer to $L^p(\Omega), 1 \leq p < \infty$, as the Banach space of p-th power Lebesgue integrable functions on Ω with norm $\|\cdot\|_{0,p,\Omega}$ and to $L^\infty(\Omega)$ as the Banach space of essentially bounded functions on Ω with norm $\|\cdot\|_{0,\infty,\Omega}$. Given a Muckenhoupt weight function ω of class $\mathcal{A}_p, 1 \leq p < \infty$, [23, 27], the space $L^p(\Omega;\omega)$ is the Banach space of weighted p-th power Lebesgue integrable functions u on Ω with norm $\|u\|_{0,p,\omega,\Omega} := (\int_\Omega \omega |u|^p \ dx)^{1/p}$.
Further, we denote by $W^{s,p}(\Omega), s \in \mathbb{R}_+, 1 \leq p \leq \infty$, the Sobolev spaces with norms $\|\cdot\|_{s,p,\Omega}$. We note that for $p = 2$ the spaces $L^2(\Omega)$ and $W^{s,2}(\Omega) = H^s(\Omega)$ are Hilbert spaces with inner products $(\cdot,\cdot)_{0,2,\Omega}$ and $(\cdot,\cdot)_{s,2,\Omega}$. In the sequel, we will suppress the subindex 2 and write $(\cdot,\cdot)_{0,\Omega}, (\cdot,\cdot)_{s,\Omega}$ and $\|\cdot\|_{0,\Omega}, \|\cdot\|_{s,\Omega}$ instead of $(\cdot,\cdot)_{0,2,\Omega}, (\cdot,\cdot)_{s,2,\Omega}$ and $\|\cdot\|_{0,2,\Omega}, \|\cdot\|_{s,2,\Omega}$.
Moreover, for a Muckenhoupt weight function ω of class $\mathcal{A}_1$ we denote by $BV(\Omega;\omega)$ the Banach space of functions $u \in L^1(\Omega;\omega)$ such that

$$\mathrm{var}_\omega u(\Omega) := \sup \ \{-\int_\Omega u\nabla\cdot\mathbf{q} \ dx, \mathbf{q} \in C_0^1(\Omega;\mathbb{R}^2), |\mathbf{q}| \leq \omega \text{ in } \Omega\} < \infty,$$

equipped with the norm

$$\|u\|_{BV(\Omega;\omega)} := \|u\|_{0,1,\omega,\Omega} + \mathrm{var}_\omega u(\Omega).$$

2. The Kobayashi-Warren-Carter system

The Kobayashi-Warren-Carter system is an orientation field based multi-phase field approach where the associated free energy functional is given in terms of an orientation field Θ, which locally describes the crystallographic orientation, and a structural order parameter ϕ, which is called the orientation order and describes the local degree of crystallinity. For a bounded convex domain Ω with boundary $\Gamma = \partial\Omega$ the free energy reads as follows:

$$F(\Theta,\phi)) = \int_\Omega \Big(s(\nabla\phi,\Theta)^2 \ |\nabla\phi|^2 + g(\phi)\Big) \ dx + H\int_\Omega \omega(\phi)|\nabla\Theta| \ dx. \tag{2.1}$$

Here, the function $s = s(\boldsymbol{\eta}, \gamma), \boldsymbol{\eta} = (\eta_1, \eta_2)^T \in \mathbb{R}^2, \gamma \in \mathbb{R}$, refers to the anisotropy function

$$s(\boldsymbol{\eta}, \gamma) = 1 + s_0 \cos(m_S \vartheta - 2\pi\gamma), \tag{2.2a}$$

$$\vartheta = \begin{cases} \pi/2 \ , \text{ if } \eta_1 = 0, \\ \arctan(\chi_{\varepsilon_a}(\eta_2/\eta_1)) \ , \text{ otherwise} \end{cases}, \tag{2.2b}$$

where $0 \leq s_0 \ll 1$ is the amplitude of the anisotropy of the interfacial free energy, m_S is the symmetry index (e.g., $m_S = 4$ for fourfold symmetry), and $\chi_{\varepsilon_a} \in C^2(\mathbb{R}), 0 < \varepsilon_a \leq 1$, is a smooth approximation of $\chi(x) = |x|, x \in \mathbb{R}$, with $\chi_{\varepsilon_a}(x) = \chi(x), |x| \geq \varepsilon_a$, $\chi'_{\varepsilon_a}(\pm\varepsilon_a) = \pm 1, \chi''_{\varepsilon_a}(\pm\varepsilon_a) = 0$, and $\chi_{\varepsilon_a}(0) = 0$, e.g., we may choose

$$\chi_{\varepsilon_a}(x) = \begin{cases} |x| \ , \ |x| \geq \varepsilon_a \\ \frac{15}{8}\varepsilon_a^{-1} x^2 - \frac{5}{4}\varepsilon_a^{-3} x^4 + \frac{3}{8}\varepsilon_a^{-5} x^6 \ , \ |x| \leq \varepsilon_a \end{cases}. \tag{2.3}$$

We note that ϑ is related to the inclination of the normal vector of the interface in the laboratory frame. The constant $H > 0$ stands for the free energy of the low-grain boundaries. The function g is the quartic double-well function

$$g(\eta) = \frac{1}{4} \eta^2 \ (1 - \eta)^2, \tag{2.4}$$

and the function ω is given by

$$\omega(\eta) = \begin{cases} \varepsilon_r \ , \ \eta \leq 0 \\ \varepsilon_r + 2(2 - 3\varepsilon_r)\eta^2 - 4(1 - \varepsilon_r)\eta^3 + \eta^4 \ , \ 0 \leq \eta \leq 1 \\ 1 - \varepsilon_r \ , \ \eta \geq 1 \end{cases}, \ \eta \in \mathbb{R}, \tag{2.5}$$

where $0 < \varepsilon_r \ll 1$, interpolating between $(0, \varepsilon_r)$ and $(1, 1 - \varepsilon_r)$. Moreover, the constant $H > 0$ stands for the free energy of the low-angle grain boundaries. The functions g and ω have the following properties

$$g(\eta) \geq 0, \quad \eta \in \mathbb{R}, \tag{2.6a}$$

$$\varepsilon_r \leq \omega(\eta) \leq 1 - \varepsilon_r, \quad \eta \in \mathbb{R}. \tag{2.6b}$$

The second integral in (2.1) has to be interpreted as the weighted total variation

$$\int\limits_{\Omega} \omega(\phi)|\nabla\Theta| \ dx = \mathrm{var}_\omega \Theta(\Omega), \quad \Theta \in BV(\Omega; \omega). \tag{2.7}$$

We note that the contribution of Θ to the free energy gives rise to a second order total variation flow. An appropriate way to handle the difficulties associated with that term is to provide a regularization by means of a regularization parameter $0 < \kappa_\Theta \ll 1$, i.e., instead of (2.1) we consider the regularized free energy

$$F(\Theta, \phi) = \int\limits_{\Omega} \Big(s(\nabla\phi, \Theta)^2 \ |\nabla\phi|^2 + g(\phi) \Big) \ dx + H \int\limits_{\Omega} \omega(\phi)(\kappa_\Theta + |\nabla\Theta|^2)^{1/2} \ dx. \tag{2.8}$$

For the second integral in (2.8) we have (cf. [1, 10] for BV functions):

(2.9)

$$\int_\Omega \omega(\phi)(\kappa_\Theta + |\nabla\Theta|^2)^{1/2}\ dx = \mathrm{var}_\omega^{(\kappa_\Theta)}\Theta(\Omega), \quad \Theta \in BV(\Omega;\omega),$$

$$\mathrm{var}_\omega^{(\kappa_\Theta)}\Theta(\Omega) :=$$

$$\sup\{\int_\Omega (-\Theta\nabla\cdot\mathbf{q} + \kappa_\Theta^{1/2}(\omega(\phi) - |\mathbf{q}|^2)^{1/2}\ dx,\ \mathbf{q} \in C_0^1(\Omega;\mathbb{R}^2),\ |\mathbf{q}| \le \omega(\phi) \text{ in } \Omega\}.$$

We split the regularized free energy (2.8) according to

$$F(\Theta,\phi) = F^{(1)}(\Theta,\phi) + F^{(2)}(\Theta,\phi), \tag{2.10}$$

$$F^{(1)}(\Theta,\phi) := \int_\Omega \Big(s(\nabla\phi,\Theta)^2\ |\nabla\phi|^2 + g(\phi)\Big)\ dx,$$

$$F^{(2)}(\Theta,\phi) := H\mathrm{var}_\omega^{(\kappa_\Theta)}\Theta(\Omega).$$

Denoting by $M_\phi > 0$ and $M_\Theta > 0$ the mobilities associated with the phase field variables ϕ and Θ, the dynamics of the crystallization process are given by the evolution inclusion

$$\frac{\partial\Theta}{\partial t} + M_\Theta \frac{\delta F^{(1)}}{\delta\Theta}(\Theta,\phi) \in -M_\Theta\ \partial_\Theta F^{(2)}(\Theta,\phi), \tag{2.11a}$$

and the evolution equation

$$\frac{\partial\phi}{\partial t} = -M_\phi\ \frac{\delta F}{\delta\phi}(\Theta,\phi). \tag{2.11b}$$

Here, $\frac{\delta F^{(1)}}{\delta\Theta}$ and $\frac{\delta F}{\delta\phi}$ are the partial Gâteaux derivatives of $F^{(1)}$ and F with respect to Θ and ϕ, whereas $\partial_\Theta F^{(2)}$ stands for the subdifferential of $F^{(2)}$ with respect to Θ.

The phase field model (2.11a),(2.11b) can be formally written as an initial-boundary value problem for a system of evolutionary partial differential equations consisting of two nonlinear second order parabolic equations in Θ and ϕ. We set $a(\boldsymbol{\eta},\gamma) = (a_{ij}(\boldsymbol{\eta},\gamma))_{i,j=1}^2$ with

(2.12)

$$a_{11}(\boldsymbol{\eta},\gamma) = a_{22}(\boldsymbol{\eta},\gamma) = s(\boldsymbol{\eta},\gamma)^2, \quad a_{12}(\boldsymbol{\eta},\gamma) = -a_{21}(\boldsymbol{\eta},\gamma) = -s(\boldsymbol{\eta},\gamma)\frac{\partial s(\boldsymbol{\eta},\gamma)}{\partial\vartheta}.$$

We further define

$$z(\phi,\Theta) := M_\Theta s(\nabla\phi,\Theta)\frac{\partial s(\nabla\phi,\Theta)}{\partial\Theta}, \tag{2.13}$$

$$r(\phi,\Theta) := g'(\phi) + \omega'(\phi)H(\kappa_\Theta + |\nabla\Theta|^2)^{1/2}.$$

Setting $Q := \Omega\times(0,T)$, $\Sigma := \Gamma\times(0,T)$, where $T > 0$ is the final time, and specifying appropriate boundary conditions and initial conditions for all phase field variables, the initial-boundary problem reads

$$\frac{\partial\Theta}{\partial t} = M_\Theta H \nabla\cdot(\omega(\phi)(\kappa_\Theta + |\nabla\Theta|^2)^{-1/2}\nabla\Theta) + z(\phi,\Theta)|\nabla\phi|^2, \tag{2.14a}$$

$$\frac{\partial\phi}{\partial t} = M_\phi \nabla\cdot(a(\nabla\phi,\Theta)\nabla\phi) - M_\phi r(\phi,\Theta), \quad \text{in } Q \tag{2.14b}$$

$$\mathbf{n}_\Gamma\cdot\omega(\phi)(\kappa_\Theta + |\nabla\Theta|^2)^{-1/2}\nabla\Theta = 0 \quad \text{on } \Sigma, \tag{2.14c}$$

$$\mathbf{n}_\Gamma\cdot a(\nabla\phi,\Theta)\nabla\phi = 0 \quad \text{on } \Sigma, \tag{2.14d}$$

$$\Phi(\cdot,0) = \Phi^0,\ \Theta(\cdot,0) = \Theta^0 \text{ in } \Omega. \tag{2.14e}$$

A weak solution of (2.14a)-(2.14e) is a pair (Θ,ϕ) with

$$\Theta \in W^{1,1}(\Omega)\cap L^\infty(\Omega), \qquad \frac{\partial\Theta}{\partial t} \in L^2(\Omega), \tag{2.15a}$$

$$\phi \in W^{1,2}(\Omega)\cap L^\infty(\Omega), \quad \frac{\partial\phi}{\partial t} \in L^2(\Omega), \tag{2.15b}$$

such that for all

$$v_1 \in W^{1,1}(\Omega)\cap L^\infty(\Omega), \quad v_2 \in W^{1,2}(\Omega)\cap L^\infty(\Omega)$$

it holds

$$\int_\Omega \frac{\partial\Theta}{\partial t} v_1\ dx + H\int_\Omega M_\Theta \omega(\phi)(\kappa_\Theta + |\nabla\Theta|^2)^{-1/2}\nabla\Theta\cdot\nabla v_1\ dx - \int_\Omega z(\phi,\Theta)|\nabla\phi|^2 v_1\ dx = 0, \tag{2.16a}$$

$$\int_\Omega \frac{\partial\phi}{\partial t} v_2\ dx + \int_\Omega M_\phi\Big(a(\nabla\phi,\Theta)\nabla\phi\cdot\nabla v_2 + r(\phi,\Theta)v_2\Big)\ dx = 0. \tag{2.16b}$$

Remark 2.1. *The mobilities M_Θ and M_ϕ may depend on ϕ according to*

$$M_\phi = M(\phi) = M_0(1-\omega(\phi)), \quad M_0 > 0, \tag{2.17a}$$

$$M_\Theta(\phi) = \chi M(\phi), \quad \chi = 0.5 \text{ or } \chi = 0.05. \tag{2.17b}$$

In this case, we replace M_Θ in (2.16a) by $M_\Theta(\phi)$ and M_ϕ in (2.16b) by $M(\phi)$.

3. The splitting scheme

We consider a discretization in time with respect to a partition of the time interval $[0,T]$ into subintervals $[t_{m-1},t_m], 1\le m\le M, M\in\mathbb{N}$, of length $\tau_m := t_m - t_{m-1}$. We denote by Θ^m and ϕ^m approximations of Θ and ϕ at time t_m and discretize (2.16) implicitly in time by the backward Euler method: Given $\Theta^{m-1}\in BV(\Omega;\omega(\phi^{m-1}))$ and $\phi^{m-1}\in W^{1,2}(\Omega), 1\le m\le M$, compute $\Theta^m \in BV(\Omega;\omega(\phi^m))$ and $\phi^m\in W^{1,2}(\Omega)$ such that it holds

$$\Theta^m - \Theta^{m-1} + M_\Theta\tau_m\frac{\delta F^{(1)}}{\delta\Theta}(\Theta^m,\phi^m) \in -M_\Theta\partial_\Theta F^{(2)}(\Theta^m,\phi^m), \tag{3.1a}$$

$$\phi^m - \phi^{m-1} = -M_\phi\tau_m\frac{\delta F}{\delta\phi}(\Theta^m,\phi^m). \tag{3.1b}$$

The splitting scheme for the solution of (3.1) is such that we first compute $\Theta^m \in V$ as the solution of

$$\Theta^m - \Theta^{m-1} + M_\Theta \tau_m \frac{\delta F^{(1)}}{\delta \Theta}(\Theta^m, \phi^{m-1}) \in -M_\Theta \tau_m \partial_\Theta F^{(2)}(\Theta^m, \phi^{m-1}), \tag{3.2a}$$

and then compute $\phi^m \in W^{1,2}(\Omega)$ satisfying

$$\phi^m - \phi^{m-1} = -M_\phi \tau_m \frac{\delta F}{\delta \phi}(\Theta^m, \phi^m). \tag{3.2b}$$

We will prove that both (3.2a) and (3.2b) have a solution by showing that the equations are the necessary optimality conditions of unconstrained minimization problems admitting local minimizers. We begin with (3.2a) and we introduce the energy functional

$$\begin{aligned} F_1^{m,\tau_m}(\Theta) &:= \frac{1}{2}\|\Theta - \Theta^{m-1}\|_{0,\Omega}^2 + \tau_m \ F_1(\Theta, \phi^{m-1}), \\ F_1(\Theta, \phi^{m-1}) &:= H M_\Theta \ \mathrm{var}_{\omega(\phi^{m-1})}^{(\kappa_\Theta)} \Theta(\Omega) + \\ & M_\Theta \int_\Omega \Big(s(\nabla \phi^{m-1}, \Theta)^2 |\nabla \phi^{m-1}|^2 + g(\phi^{m-1}) \Big) \ dx. \end{aligned} \tag{3.3}$$

Theorem 3.1. *The energy functional $F_1^{m,\tau_m} : V \to \mathbb{R}$ has a local minimizer $\Theta^m \in V$, i.e.,*

$$F_1^{m,\tau_m}(\Theta^m) = \inf_{\Theta \in V} F_1^{m,\tau_m}(\Theta). \tag{3.4}$$

Proof. We first show that the energy functional F_1^{m,τ_m} is coercive on V. We have

$$\frac{1}{2}\|\Theta - \Theta^{m-1}\|_{0,\Omega}^2 \geq \frac{1}{4}\|\Theta\|_{0,\Omega}^2 - \frac{1}{2}\|\Theta^{m-1}\|_{0,\Omega}^2. \tag{3.5}$$

Moreover, observing (2.2), we get

$$M_\Theta \int_\Omega s(\nabla \phi^{m-1}, \Theta)^2 |\nabla \phi^{m-1}|^2 \ dx \geq M_\Theta (1 - s_0)^2 \|\nabla \phi^{m-1}\|_{0,\Omega}^2. \tag{3.6}$$

Combining (3.5) and (3.6) gives

$$\begin{aligned} F_1^{m,\tau_m}(\Theta) \geq & \frac{1}{4}\|\Theta\|_{0,\Omega}^2 + H M_\Theta \tau_m \ \mathrm{var}_{\omega(\phi^{m-1})}^{(\kappa_\Theta)} \Theta(\Omega) + \\ & M_\Theta (1 - s_0)^2 \tau_m \|\nabla \phi^{m-1}\|_{0,\Omega}^2 + M_\Theta \tau_m \int_\Omega g(\phi^{m-1}) \ dx - \frac{1}{2}\|\Theta^{m-1}\|_{0,\Omega}^2, \end{aligned} \tag{3.7}$$

from which we conclude, observing $BV(\Omega; \omega(\phi^{m-1})) \subset L^2(\Omega; \omega(\phi^{m-1})) \subset L^2(\Omega)$ and $\mathrm{var}_{\omega(\phi^{m-1})}^{(\kappa_\Theta)} \Theta(\Omega) \geq \mathrm{var}_{\omega(\phi^{m-1})} \Theta(\Omega)$.

The functional $F_1(\Theta, \phi^{m-1})$ is not convex in Θ. We split it according to

$$F_1(\Theta, \phi^{m-1}) = F_{1,1}(\Theta, \phi^{m-1}) + F_{1,2}(\Theta, \phi^{m-1}),$$

where $F_{1,1}(\Theta, \phi^{m-1})$ and $F_{1,2}(\Theta, \phi^{m-1})$ are given by

$$\begin{aligned} F_{1,1}(\Theta, \phi^{m-1}) &:= H M_\Theta \ \mathrm{var}_{\omega(\phi^{m-1})}^{(\kappa_\Theta)} \Theta(\Omega), \\ F_{1,2}(\Theta, \phi^{m-1}) &:= M_\Theta \int_\Omega \Big(s(\nabla \phi^{m-1}, \Theta)^2 |\nabla \phi^{m-1}|^2 + g(\phi^{m-1}) \Big) \ dx, \end{aligned}$$

and we define

$$F_{1,1}^{m,\tau_m}(\Theta) := \frac{1}{2}\|\Theta - \Theta^{m-1}\|_{0,\Omega}^2 + \tau_m\ F_{1,1}(\Theta, \phi^{m-1}). \tag{3.8}$$

To prove the existence of a local minimizer, let $(\Theta_n)_{n\in\mathbb{N}}, \Theta_n \in V, n \in \mathbb{N}$, be a minimizing sequence. Due to the coercivity of $F_{1,1}^{m,\tau_m}$, the sequence is bounded and hence, there exist $\mathbb{N}' \subset \mathbb{N}$ and $\Theta^m \in V$ such that for $\mathbb{N}' \ni n \to \infty$ it holds (cf. Theorem 5.1 in [2])

$$\Theta_n \to \Theta^m \text{ in } L^q(\Omega, \omega(\phi^{m1})), 1 \le q < 2, \tag{3.9a}$$

$$\Theta_n \rightharpoonup \Theta^m \text{ in } L^2(\Omega). \tag{3.9b}$$

In view of (3.9a) we have the following semicontinuity property (cf. Theorem 3.2 in [2])

$$\mathrm{var}_{\omega(\phi^{m-1})}^{(\kappa_\Theta)}\Theta^m(\Omega) \le \lim \inf_{\mathbb{N}'\ni n\to\infty} \mathrm{var}_{\omega(\phi^{m-1})}^{(\kappa_\Theta)}\Theta_n(\Omega). \tag{3.10}$$

Further, it follows from (3.9b) that

$$\|\Theta^m - \Theta^{m-1}\|_{0,\Omega}^2 \le \lim \inf_{\mathbb{N}'\ni n\to\infty} \|\Theta_n - \Theta^{m-1}\|_{0,\Omega}^2. \tag{3.11}$$

Due to the continuity of s we also have

$$M_\Theta s(\nabla\phi^{m-1}, \Theta_n)^2 \to M_\Theta s(\nabla\phi^{m-1}, \Theta^m)^2$$

almost everywhere in Ω as $\mathbb{N}'' \ni n \to \infty$.
Moreover, the sequence $\{M_\Theta s(\nabla\phi^{m-1}, \Theta_n)^2|\nabla\phi^{m-1}|^2\}_{n\in\mathbb{N}''}$ is uniformly integrable and $M_\Theta s(\nabla\phi^{m-1}, \Theta^m)^2|\nabla\phi^{m-1}|^2 \in L^1(\Omega)$. The Vitali convergence theorem (cf., e.g., [26]) yields

$$F_{1,2}(\Theta^m, \phi^{m-1}) = \lim_{\mathbb{N}''\ni n\to\infty} F_{1,2}(\Theta_n, \phi^{m-1}). \tag{3.12}$$

Hence, (3.10)-(3.12) imply

$$F_1^{m,\tau_m}(\Theta^m) \le \lim \inf_{n\to\infty} F_1^{m,\tau_m}(\Theta_n), \tag{3.13}$$

which allows to conclude. □

Next, we consider the energy functional

$$F_2^{m,\tau_m}(\phi) := \frac{1}{2}\ \|\phi - \phi^{m-1}\|_{0,\Omega}^2 + \tau_m F_2(\Theta^m, \phi), \tag{3.14}$$

$$F_2(\Theta^m, \phi)) := M_\phi \int_\Omega \Big(s(\nabla\phi, \Theta^m)^2\ |\nabla\phi|^2 + g(\phi)\Big)\ dx + HM_\phi\ \mathrm{var}_{\omega(\phi^m)}^{(\kappa_\Theta)}\Theta^m(\Omega).$$

Theorem 3.2. *For sufficiently small $s_0 > 0$, the energy functional $F_2^{m,\tau_m} : W^{1,2}(\Omega) \to \mathbb{R}$ has a local minimizer $\phi^m \in W^{1,2}(\Omega)$, i.e.,*

$$F_2^{m,\tau_m}(\phi^m) = \inf_{\phi\in W^{1,2}(\Omega)} F_2^{m,\tau_m}(\phi). \tag{3.15}$$

Proof. We first show that the functional F_2^{m,τ_m} is coercive on $W^{1,2}(\Omega)$: By Young's inequality we find

$$\frac{1}{2}\ \|\phi - \phi^{m-1}\|_{0,\Omega}^2 \geq \frac{1}{4}\ \|\phi\|_{0,\Omega}^2 - \frac{1}{2}\ \|\phi^{m-1}\|_{0,\Omega}^2. \tag{3.16}$$

Further, we take advantage of (2.6) to conclude

$$F_2^{m,\tau_m}(\phi) \geq M_\phi \varepsilon_r (1-s_0)^2 \tau_m \|\nabla\phi\|_{0,\Omega}^2 + \frac{1}{4}\|\phi\|_{0,\Omega}^2 - \frac{1}{2}\ \|\phi^{m-1}\|_{0,\Omega}^2. \tag{3.17}$$

The functional $F_2(\Theta^m, \phi)$ is not convex in ϕ, but it can be split into a convex part $F_{2,1}(\Theta^m, \phi)$ and non-convex part $F_{2,2}(\Theta^m, \phi)$ according to

$$F_{2,1}(\Theta^m, \phi) := \frac{1}{2}\ \|\phi - \phi^{m-1}\|_{0,\Omega}^2 + \tau_m M_\phi \int_\Omega s(\nabla\phi, \Theta^m)^2 |\nabla\phi|^2\ dx,$$

$$F_{2,2}(\Theta^m, \phi) := M_\phi \int_\Omega g(\phi)\ dx + M_\phi \mathrm{var}_{\omega(\phi^m)}^{(\kappa_\Theta)} \Theta^m(\Omega).$$

The convexity of the first part $\|\phi - \phi^{m-1}\|_{0,\Omega}^2/2$ of $F_{2,1}(\Theta^m, \phi)$ is obvious. As far as the convexity of the second part is concerned, for fixed $\gamma \in \mathbb{R}$ we define $g_1 \in C^2(\mathbb{R}^2)$ by

$$g_1(\eta) := (1 + s_0 \cos(m_S \vartheta - 2\pi\gamma)))^2 (\eta_1^2 + \eta_2^2), \quad \eta = (\eta_1, \eta_2) \in \mathbb{R}^2,$$

where ϑ is given by (2.2b). Computing the second partial derivatives $\partial^2 g_1/\partial\eta_i^2, 1 \leq i \leq 2$, and $\partial^2 g_1/(\partial\eta_1\partial\eta_2)$, it can be shown that for sufficiently small s_0 the Hessian of g_1 is positive definite, i.e., there exists $\alpha > 0$ such that

$$\sum_{i,j=1}^{2} \frac{\partial^2 g_1}{\partial\eta_i \partial\eta_j} \xi_i \xi_j \geq \alpha |\xi|^2 \quad \text{for all } \xi = (\xi_1, \xi_2)^T \in \mathbb{R}^2.$$

In order to prove the existence of a local minimizer let $\{\phi_n\}_{\mathbb{N}}, \phi_n \in W^{1,2}(\Omega)$, be a minimizing sequence, i.e., it holds

$$F_2^{m,\tau_m}(\phi_n) \to \inf_{\phi \in W^{1,2}(\Omega)} F_2^{m,\tau_m}(\phi) \quad (n \to \infty). \tag{3.18}$$

Due to the coercivity of F_2^{m,τ_m} the sequence $\{\phi_n\}_{\mathbb{N}}$ is bounded in $W^{1,2}(\Omega)$. Hence, there exists a weakly convergent subsequence, i.e., there exist $\mathbb{N}' \subset \mathbb{N}$ and $\phi^m \in W^{1,2}(\Omega)$ such that $\phi_n \rightharpoonup \phi^m$ $(\mathbb{N}' \ni n \to \infty)$ in $W^{1,2}(\Omega)$. The Rellich-Kondrachev theorem implies strong convergence in $L^p(\Omega)$ for any $1 \leq p < \infty$ and hence, for some subsequence $\mathbb{N}'' \subset \mathbb{N}'$ we have

$$\phi_n \to \phi^m \quad \text{almost everywhere in } \Omega \text{ as } \mathbb{N}'' \ni n \to \infty.$$

Due to the continuity of g and ω, we also have

$$g(\phi_n) \to g(\phi^m) \quad \text{almost everywhere in } \Omega \text{ as } \mathbb{N}'' \ni n \to \infty,$$

$$\omega(\phi_n) \to \omega(\phi^m) \quad \text{almost everywhere in } \Omega \text{ as } \mathbb{N}'' \ni n \to \infty.$$

The sequence $\{M_\phi g(\phi_n)\}_{n \in \mathbb{N}''}$ is uniformly integrable and $M_\phi g(\phi^m) \in L^1(\Omega)$. Again, the Vitali convergence theorem implies

$$M_\phi \int_\Omega g(\phi_n)\ dx \to M_\phi \int_\Omega g(\phi^m)\ dx \quad \text{as } \mathbb{N}'' \ni n \to \infty. \tag{3.19}$$

Moreover, since $\omega(\phi_n) \to \omega(\phi^m)$ almost everywhere in Ω as $\mathbb{N}'' \ni n \to \infty$, we have

$$\text{var}_{\omega(\phi_n)}^{(\kappa_\Theta)} \Theta^m(\Omega) \to \text{var}_{\omega(\phi^m)}^{(\kappa_\Theta)} \Theta^m(\Omega) \quad \text{as } \mathbb{N}'' \ni n \to \infty. \tag{3.20}$$

Obviously, the functional $F_{2,1}(\Theta^m, \cdot)$ is continuous on $W^{1,2}(\Omega)$ and thus lower semicontinuous. As we have shown before, it is convex and hence, it is weakly lower semicontinuous. This gives

$$F_{2,1}(\Theta^m, \phi^m) \leq \liminf_{\mathbb{N}'' \ni n \to \infty} F_{2,1}(\Theta^m, \phi_n). \tag{3.21}$$

Now, (3.18),(3.19),(3.20), and (3.21) imply that (3.15) holds true. □

We show that each time step the splitting scheme leads to a decrease of the regularized free energy.

Theorem 3.3. *The splitting scheme is energy stable with respect to the regularized free energy* (2.8)*, i.e., it holds*

$$F(\Theta^m, \phi^m) \leq F(\Theta^{m-1}, \phi^{m-1}), \quad m \geq 1. \tag{3.22}$$

Proof. From Theorem 3.1 and Theorem 3.2 we deduce

$$\begin{aligned} F_1^{m,\tau_m}(\Theta^m) &= \frac{1}{2}\|\Theta^m - \Theta^{m-1}\|_{0,\Omega}^2 + \tau_m F_1(\Theta^m, \phi^{m-1}) \\ &\leq F_1^{m,\tau_m}(\Theta^{m-1}) = \tau_m F_1(\Theta^{m-1}, \phi^{m-1}), \end{aligned} \tag{3.23a}$$

$$\begin{aligned} F_2^{m,\tau_m}(\phi^m) &= \frac{1}{2}\|\phi^m - \phi^{m-1}\|_{0,\Omega}^2 + \tau_m F_2(\Theta^m, \phi^m) \\ &\leq F_2^{m,\tau_m}(\phi^{m-1}) = \tau_m F_2(\Theta^m, \phi^{m-1}). \end{aligned} \tag{3.23b}$$

Moreover, in view of (2.10),(3.3), and (3.14) we have

(3.24a)
$$F_1(\Theta^m, \phi^{m-1}) = M_\Theta F(\Theta^m, \phi^{m-1})) \quad \text{and} \quad F_2(\Theta^m, \phi^{m-1}) = M_\phi F(\Theta^m, \phi^{m-1})),$$

(3.24b)
$$F_1(\Theta^{m-1}, \phi^{m-1}) = M_\Theta F(\Theta^{m-1}, \phi^{m-1})) \quad \text{and} \quad F_2(\Theta^m, \phi^m) = M_\phi F(\Theta^m, \phi^m)).$$

From (3.24a) we deduce that

$$F_1(\Theta^m, \phi^{m-1}) = \frac{M_\Theta}{M_\phi} F_2(\Theta^m, \phi^{m-1}). \tag{3.25}$$

It follows from (3.23a),(3.23b), and (3.25) that

$$\begin{aligned} &\tau_m F_2(\Theta^m, \phi^m) \leq F_2^{m,\tau_m}(\phi^m) \leq \tau_m F_2(\Theta^m, \phi^{m-1}) \ = \\ &\tau_m \frac{M_\phi}{M_\Theta} F_1(\Theta^m, \phi^{m-1}) = \frac{M_\phi}{M_\Theta}\Big(F_1^{m,\tau_m}(\Theta^m) - \frac{1}{2}\|\Theta^m - \Theta^{m-1}\|_{0,\Omega}^2\Big) \ \leq \\ &\frac{M_\phi}{M_\Theta} F_1^{m,\tau_m}(\Theta^m) \leq \tau_m \frac{M_\phi}{M_\Theta} F_1(\Theta^{m-1}, \phi^{m-1}). \end{aligned} \tag{3.26}$$

In view of (3.24b), (3.22) is a consequence of (3.26). □

Remark 3.1. *Theorem 3.1 and Theorem 3.2 provide the existence of a solution of the splitting scheme, but do not imply uniqueness due to the presence of the nonconvex parts $F_{1,2}(\Theta, \phi^{m-1})$ and $F_{2,2}(\Theta^m, \phi)$ of $F_1^{m,\tau_m}(\Theta)$ and $F_2^{m,\tau_m}(\phi)$. However, for related problems such as the Allen-Cahn and the Cahn-Hilliard equation, epitaxial thin film models, and the phase field crystal equation, convex-concave splittings* *of the energy functionals have been suggested that guarantee both uniqueness of a solution and energy stability (cf.* [3, 4, 8, 9] *and the references therein). Similar convex-concave splittings*

$$F_{1,2}(\Theta,\phi^{m-1}) = \tilde{F}_{1,2}(\Theta,\phi^{m-1}) + \hat{F}_{1,2}(\Theta,\phi^{m-1}),$$
$$F_{2,2}(\Theta^m,\phi) = \tilde{F}_{2,2}(\Theta^m,\phi) + \hat{F}_{2,2}(\Theta^m,\phi)$$

into strongly convex parts $\tilde{F}_{1,2}(\Theta,\phi^{m-1}), \tilde{F}_{2,2}(\Theta^m,\phi)$ *and concave parts* $\hat{F}_{1,2}(\Theta,\phi^{m-1}), \hat{F}_{2,2}(\Theta^m,\phi)$ *can be applied here as well according to*

$$\tilde{F}_{1,2}(\Theta,\phi^{m-1}) = F_{1,2}(\Theta,\phi^{m-1}) + G_{1,2}(\Theta,\phi^{m-1}),\ \hat{F}_{1,2}(\Theta,\phi^{m-1}) = -G_{1,2}(\Theta,\phi^{m-1}),$$
$$\tilde{F}_{2,2}(\Theta^m,\phi) = F_{2,2}(\Theta^m,\phi) + G_{2,2}(\Theta^m,\phi),\ \hat{F}_{2,2}(\Theta^m,\phi) = -G_{2,2}(\Theta^m,\phi),$$

where $G_{1,2}(\Theta,\phi^{m-1})$ *and* $G_{2,2}(\Theta^m,\phi)$ *are appropriately chosen strongly convex functions in* Θ *and* ϕ*, respectively. The splitting scheme based on the convex-concave decomposition reads*

$$\Theta^m - \Theta^{m-1} + M_\Theta\tau_m \frac{\delta\tilde{F}_{1,2}}{\delta\Theta}(\Theta^m,\phi^{m-1}) \ \in$$
$$- M_\Theta\tau_m\partial_\Theta F^{(2)}(\Theta^m,\phi^{m-1}) - M_\Theta\tau_m\frac{\delta\hat{F}_{1,2}}{\delta\Theta}(\Theta^{m-1},\phi^{m-1}),$$
$$\phi^m - \phi^{m-1} + M_\phi\tau_m\frac{\delta(F_{2,1}+\tilde{F}_{2,2})}{\delta\phi}(\Theta^m,\phi^m) = -M_\phi\tau_m\frac{\delta\hat{F}_{2,2}}{\delta\phi}(\Theta^m,\phi^{m-1}).$$

For sufficiently smooth time-discrete phase field varibales Θ^m and ϕ^m, the optimality conditions (3.1a),(3.1b) can be written as the following two individual elliptic boundary value problems

(3.27a)
$$\Theta^m - HM_\Theta\tau_m\nabla\cdot(\omega(\phi^{m-1})(\kappa_\Theta + |\nabla\Theta^m|^2)^{-1/2}\nabla\Theta^m) - \tau_m z(\phi^{m-1},\Theta^m)|\nabla\Theta^m|^2 = \Theta^{m-1} \quad \text{in } \Omega,$$

(3.27b)
$$\mathbf{n}_\Gamma\cdot(\omega(\phi^{m-1})(\kappa_\Theta + |\nabla\Theta^m|^2)^{-1/2}\nabla\Theta^m) = 0 \quad \text{on } \Gamma,$$

and

(3.28a)
$$\phi^m - M_\phi\tau_m\nabla\cdot(a(\nabla\phi^m,\Theta^m)\nabla\phi^m) + M_\phi\tau_m r(\phi^m,\Theta^m) = \phi^{m-1} \quad \text{in } \Omega,$$

(3.28b)
$$\mathbf{n}_\Gamma\cdot a(\nabla\phi^m,\Theta^m)\nabla\phi^m = 0 \quad \text{on } \Gamma.$$

A weak solution of (3.27a),(3.27b), and (3.28a),(3.28b) is a pair (Θ^m,ϕ^m) with $\Theta^m \in W^{1,1}(\Omega)\cap L^\infty(\Omega)$ and $\phi^m \in W^{1,2}(\Omega)\cap L^\infty(\Omega)$ such that for all $v_1 \in W^{1,1}(\Omega)\cap$

$L^\infty(\Omega)$ and $v_2 \in W^{1,2}(\Omega) \cap L^\infty(\Omega)$ it holds

$$(\Theta^m, v_1)_{0,\Omega} + H\tau_m \int_\Omega M_\Theta \omega(\phi^{m-1})(\kappa_\Theta + |\nabla\Theta^m|^2)^{-1/2} \nabla\Theta^m \cdot \nabla v_1 \; dx \tag{3.29a}$$

$$- \tau_m \int_\Omega z(\phi_h^{m-1}, \Theta_h^m) |\nabla \phi_h^{m-1}|^2 \; v_1 \; dx = (\Theta_h^{m-1}, v_1)_{0,\Omega},$$

$$(\phi_h^m, v_2)_{0,\Omega} + \tau_m \int_\Omega M_\phi a(\nabla\phi_h^m, \Theta_h^m) \nabla\phi_h^m \cdot \nabla v_2 \; dx \tag{3.29b}$$

$$+ \tau_m \int_\Omega M_\phi r(\phi^m, \Theta^m) \; v_2 \; dx = (\phi^{m-1}, v_2)_{0,\Omega}.$$

4. Discretization in space and numerical solution of the fully discretized system

For discretization in space of the implicitly in time discretized and split KWC system (3.2a),(3.2b) we assume $\mathcal{T}_h(\Omega)$ to be a geometrically conforming, shape regular, simplicial triangulation of the computational domain Ω. Denoting by $P_k(K), k \in \mathbb{N}, K \in \mathcal{T}_h(\Omega)$, the linear space of polynomials of degree $\le k$ on K, we refer to

$$V_h := \{v_h \in C(\bar{\Omega}) \mid v_h|_K \in P_k(K), K \in \mathcal{T}_h(\Omega)\}$$

as the finite element space of continuous piecewise polynomial Lagrangian finite elements (cf., e.g., [5]). Then, in case of variable mobilities (2.17a),(2.17b), the finite element approximation of (3.2a),(3.2b) reads as follows (cf. (3.29a),(3.29b)): Given ϕ_h^{m-1}, find $\Theta_h^m, \phi_h^m \in V_h$ such that for all $v_h \in V_h$ and $w_h \in V_h$ it holds

$$(\Theta_h^m, v_h)_{0,\Omega} + H\tau_m (M_\Theta(\phi_h^{m-1})\omega(\phi_h^{m-1})(\kappa_\Theta + |\nabla\Theta_h^m|^2)^{-1/2}\nabla\Theta_h^m, \nabla v_h)_{0,\Omega} \tag{4.1a}$$

$$- \tau_m (z(\phi_h^{m-1}, \Theta_h^m)|\nabla\phi_h^{m-1}|^2, v_h)_{0,\Omega} = (\Theta_h^{m-1}, v_h)_{0,\Omega},$$

$$(\phi_h^m, w_h)_{0,\Omega} + \tau_m (M(\phi_h^{m-1}) a(\nabla\phi_h^m, \Theta_h^m)\nabla\phi_h^m, \nabla w_h)_{0,\Omega} \tag{4.1b}$$

$$+ \tau_m (M(\phi_h^{m-1}) r(\phi_h^m, \Theta_h^m), w_h)_{0,\Omega} = (\phi_h^{m-1}, w_h)_{0,\Omega}.$$

Remark 4.1. *We note that the discrete splitting scheme* (4.1a),(4.1b) *is such that it requires the successive solution of two individual discrete elliptic equations.*

The numerical solution of (4.1a) and (4.1b) amounts to the successive solution of two nonlinear algebraic systems. We assume $V_h = \text{span}\{\varphi_1, \cdots, \varphi_{N_h}\}, N_h \in \mathbb{N}$, such that

$$\Theta_h^m = \sum_{j=1}^{N_h} \Theta_j^m \varphi_j, \quad \phi_h^m = \sum_{j=1}^{N_h} \phi_j^m \varphi_j.$$

Setting $\mathbf{\Theta}^m := (\Theta_1^m, \cdots, \Theta_{N_h}^m)^T$ and $\mathbf{\Phi}^m := (\phi_1^m, \cdots, \phi_{N_h}^m)^T$, the algebraic formulation of (4.1a) and (4.1b) leads to the two nonlinear systems

$$\mathbf{F}_1(\mathbf{\Theta}^m, \mathbf{\Phi}^{m-1}, t_m) = \mathbf{0}, \tag{4.2a}$$

$$\mathbf{F}_2(\mathbf{\Theta}^m, \mathbf{\Phi}^m, t_m) = \mathbf{0}. \tag{4.2b}$$

Here, $\mathbf{F}_k : \mathbb{R}^{N_h} \times \mathbb{R}^{N_h} \times \mathbb{R}_+ \to \mathbb{R}^{N_h}$ and the components $\mathbf{F}_{k,i}, 1 \leq i \leq N_h$, are given by

$$\mathbf{F}_{1,i}(\mathbf{\Theta}^m, \mathbf{\Phi}^{m-1}, t_m) = \sum_{j=1}^{N_h} \Theta_j^m \ (\varphi_j, \varphi_i)_{0,\Omega} +$$

$$H\tau_m \sum_{j=1}^{N_h} \Theta_j^m (M_\Theta(\mathbf{\Phi}^{m-1})\omega(\mathbf{\Phi}^{m-1})(\kappa_\Theta + |\sum_{k=1}^{N_h} \Theta_k^m \nabla\varphi_k|^2)^{-1/2} \nabla\varphi_j, \nabla\varphi_i)_{0,\Omega}$$

$$- \tau_m(z(\mathbf{\Phi}^{m-1}, \mathbf{\Theta}^m)|\sum_{k=1}^{N_h} \mathbf{\Phi}^{m-1} \nabla\varphi_k|^2, \varphi_i)_{0,\Omega} - \sum_{j=1}^{N_h} \Theta_j^{m-1} \ (\varphi_j, \varphi_i)_{0,\Omega}$$

and

$$\mathbf{F}_{2,i}(\mathbf{\Theta}^m, \mathbf{\Phi}^m, t_m) = \sum_{j=1}^{N_h} \phi_j^m \ (\varphi_j, \varphi_i)_{0,\Omega} +$$

$$\tau_m \sum_{j=1}^{N_h} \phi_j^m (M(\mathbf{\Phi}^{m-1}) a(\mathbf{\Phi}^m, \mathbf{\Theta}^m) \nabla\varphi_j, \nabla\varphi_i)_{0,\Omega} +$$

$$\tau_m(M(\mathbf{\Phi}^{m-1}) r(\mathbf{\Phi}^m, \mathbf{\Theta}^m), \varphi_i)_{0,\Omega} - \sum_{j=1}^{N_h} \phi_j^{m-1} \ (\varphi_j, \varphi_i)_{0,\Omega},$$

where

$$M_\Theta(\mathbf{\Phi}^{m-1}) := M_\Theta(\sum_{k=1}^{N_h} \phi_k^{m-1}\varphi_k), \ \ M(\mathbf{\Phi}^{m-1}) := M(\sum_{k=1}^{N_h} \phi_k^{m-1}\varphi_k),$$

$$\omega(\mathbf{\Phi}^{m-1}) := \omega(\sum_{k=1}^{N_h} \phi_k^{m-1}\varphi_k), \ \ z(\mathbf{\Phi}^{m-1}, \mathbf{\Theta}^m) := z(\sum_{k=1}^{N_h} \phi_k^{m-1}\varphi_k, \sum_{k=1}^{N_h} \Theta_k^m \varphi_k),$$

$$a(\mathbf{\Phi}^m, \mathbf{\Theta}^m) := a(\sum_{k=1}^{N_h} \phi_k^m \nabla\varphi_k, \sum_{k=1}^{N_h} \Theta_k^m \varphi_k), \ \ r(\mathbf{\Phi}^m, \mathbf{\Theta}^m) := r(\sum_{k=1}^{N_h} \phi_k^m \varphi_k, \sum_{k=1}^{N_h} \Theta_k^m \varphi_k).$$

The nonlinear systems (4.2a) and (4.2b) can be solved by Newton's method, but the problem is the appropriate choice of the time step sizes $\tau_m, 1 \leq m \leq M$, in order to guarantee convergence of Newton's method. In fact, a uniform choice $\tau_m = T/M$ only works, if M is chosen sufficiently large which would require an unnecessary huge amount of time steps. In particular, this applies to (4.2a) reflecting the singular character of the second order total variation flow problem. An appropriate way to overcome this difficulty is to consider (4.2a),(4.2b) as parameter dependent nonlinear systems with the time as a parameter and to apply a predictor corrector continuation strategy with an adaptive choice of the time steps (cf., e.g., [6, 17]). Given the pair $(\mathbf{\Theta}^{m-1}, \mathbf{\Phi}^{m-1})$, the time step size $\tau_{m-1,0} = \tau_{m-1}$, and setting $k = 0$, where k is a counter for the predictor corrector steps, the predictor step for (4.2a) consists of constant continuation leading to the initial guesses

$$\mathbf{\Theta}^{(m,k)} = \mathbf{\Theta}^{m-1}, \quad t_m = t_{m-1} + \tau_{m-1,k}. \tag{4.3}$$

Setting $\nu_1 = 0$ and $\mathbf{\Theta}^{(m,k,\nu_1)} = \mathbf{\Theta}^{(m,k)}$, for $\nu_1 \leq \nu_{max}$, where $\nu_{max} > 0$ is a pre-specified maximal number, the Newton iteration

$$\begin{aligned} \mathbf{F}'(\mathbf{\Theta}^{(m,k,\nu_1)}, \mathbf{\Phi}^{m-1}, t_m)\mathbf{\Delta\Theta}^{(m,k,\nu_1)} &= -\mathbf{F}_1(\mathbf{\Theta}^{(m,k,\nu_1)}, \mathbf{\Phi}^{m-1}, t_m), \\ \mathbf{\Theta}^{(m,k,\nu_1+1)} &= \mathbf{\Theta}^{(m,k,\nu_1)} + \mathbf{\Delta\Theta}^{(m,k,\nu_1)}, \quad \nu_1 \geq 0, \end{aligned} \tag{4.4}$$

serves as a corrector whose convergence is monitored by the contraction factor

$$\Lambda_{\Theta}^{(m,k,\nu_1)} = \frac{\|\overline{\mathbf{\Delta\Theta}^{(m,k,\nu_1)}}\|}{\|\mathbf{\Delta\Theta}^{(m,k,\nu_1)}\|}, \tag{4.5}$$

where $\overline{\mathbf{\Delta\Theta}^{(m,k,\nu_1)}}$ is the solution of the auxiliary Newton step

$$\mathbf{F}_1'(\mathbf{\Theta}^{(m,k,\nu_1)}, \mathbf{\Phi}^{m-1}, t_m)\overline{\mathbf{\Delta\Theta}^{(m,k,\nu_1)}} = -\mathbf{F}_1(\mathbf{\Theta}^{(m,k,\nu_1+1)}, \mathbf{\Phi}^{m-1}, t_m). \tag{4.6}$$

If the contraction factor satisfies

$$\Lambda_{\Theta}^{(m,k,\nu_1)} < \frac{1}{2}, \tag{4.7}$$

we set $\nu_1 = \nu_1 + 1$. If $\nu_1 > \nu_{max}$, both the Newton iteration and the predictor corrector continuation strategy are terminated indicating non-convergence. Otherwise, we continue the Newton iteration (4.4). If (4.7) does not hold true, we set $k = k + 1$ and the time step is reduced according to

$$\tau_{m,k} = \max\Big(\frac{\sqrt{2} - 1}{\sqrt{4\Lambda_{\Theta}^{(m,k,\nu_1)} + 1} - 1}\ \tau_{m,k-1}, \tau_{min}\Big), \tag{4.8}$$

where $\tau_{min} > 0$ is some pre-specified minimal time step. If $\tau_{m,k} > \tau_{min}$, we go back to the prediction step (4.3). Otherwise, the predictor corrector strategy is stopped indicating non-convergence. The Newton iteration is terminated successfully, if for some $\nu_1^* > 0$ the relative error of two subsequent Newton iterates satisfies

$$\frac{\|\mathbf{\Theta}^{(m,k,\nu_1^*)} - \mathbf{\Theta}^{(m,k,\nu_1^*-1)}\|}{\|\mathbf{\Theta}^{(m,k,\nu_1^*)}\|} < \varepsilon \tag{4.9}$$

for some pre-specified accuracy $\varepsilon > 0$. In this case, we proceed with the prediction step (4.10) below.

The predictor step for (4.2b) also consists of constant continuation leading to the initial guesses

$$\mathbf{\Phi}^{(m,k)} = \mathbf{\Phi}^{m-1}, \quad t_m = t_{m-1} + \tau_{m-1,k}. \tag{4.10}$$

Setting $\nu_2 = 0$ and $\mathbf{\Phi}^{(m,k,\nu_2)} = \mathbf{\Phi}^{(m,k)}$, for $\nu_2 \leq \nu_{max}$, the Newton iteration

$$\begin{aligned} \mathbf{F}_2'(\mathbf{\Theta}^{(m,k,\nu_1^*)}, \mathbf{\Phi}^{m,k,\nu_2}, t_m)\mathbf{\Delta\Phi}^{(m,k,\nu_2)} &= -\mathbf{F}_2(\mathbf{\Theta}^{(m,k,\nu_1^*)}, \mathbf{\Phi}^{m,k,\nu_2}, t_m), \\ \mathbf{\Phi}^{(m,k,\nu_2+1)} &= \mathbf{\Phi}^{(m,k,\nu_2)} + \mathbf{\Delta\Phi}^{(m,k,\nu_2)}, \quad \nu_2 \geq 0, \end{aligned} \tag{4.11}$$

again serves as the corrector with the convergence monitored by the contraction factor

$$\Lambda_{\phi}^{(m,k,\nu_2)} = \frac{\|\overline{\mathbf{\Delta\Phi}^{(m,k,\nu_2)}}\|}{\|\mathbf{\Delta\Phi}^{(m,k,\nu_2)}\|}, \tag{4.12}$$

where $\overline{\mathbf{\Delta\Phi}^{(m,k,\nu_2)}}$ is the solution of the auxiliary Newton step

$$\mathbf{F}_2'(\mathbf{\Theta}^{(m,k,\nu_1^*)}, \mathbf{\Phi}^{m,k,\nu_2}, t_m)\overline{\mathbf{\Delta\Phi}^{(m,k,\nu_2)}} = -\mathbf{F}_2(\mathbf{\Theta}^{(m,k,\nu_1^*)}, \mathbf{\Phi}^{m,k,\nu_2+1}, t_m). \tag{4.13}$$

If the contraction factor satisfies

$$\Lambda_\phi^{(m,k,\nu_2)} < \frac{1}{2}, \tag{4.14}$$

we set $\nu_2 = \nu_2 + 1$. If $\nu_2 > \nu_{max}$, both the Newton iteration and the predictor corrector continuation strategy are terminated indicating non-convergence. Otherwise, we continue the Newton iteration (4.11). If (4.14) is not satisfied, we set $k = k + 1$ and the time step is reduced according to

$$\tau_{m,k} = \max\Big(\frac{\sqrt{2}-1}{\sqrt{4\Lambda_\phi^{(m,\nu_2)}+1}-1}\ \tau_{m,k-1}, \tau_{min}\Big). \tag{4.15}$$

If $\tau_{m,k} > \tau_{min}$, we go back to the prediction step (4.3) for (4.2a). Otherwise, the predictor corrector strategy is stopped indicating non-convergence. The Newton iteration is terminated successfully, if for some $\nu_2^* > 0$ the relative error of two subsequent Newton iterates satisfies

$$\frac{\|\mathbf{\Phi}^{(m,k,\nu_2^*)} - \mathbf{\Phi}^{(m,k,\nu_2^*-1)}\|}{\|\mathbf{\Theta}^{(m,k,\nu_2^*)}\|} < \varepsilon. \tag{4.16}$$

In this case, we set

$$\mathbf{\Theta}^m = \mathbf{\Theta}^{(m,k,\nu_1^*)}, \quad \mathbf{\Phi}^m = \mathbf{\Phi}^{(m,k,\nu_2^*)} \tag{4.17}$$

and predict a new time step according to

(4.18)
$$\tau_m = \min\Big(\frac{(\sqrt{2}-1)\ \|\mathbf{\Delta\Theta}^{(m,k,0)}\|}{2\Lambda_\Theta^{(m,k,0)}\ \|\mathbf{\Theta}^{(m,k,0)} - \mathbf{\Theta}^m\|}, \frac{(\sqrt{2}-1)\ \|\mathbf{\Delta\Phi}^{(m,k,0)}\|}{2\Lambda_\phi^{(m,k,0)}\ \|\mathbf{\Phi}^{(m,k,0)} - \mathbf{\Phi}^m\|}, \alpha\Big)\ \tau_{m,k},$$

where $\alpha > 1$ is a pre-specified amplification factor for the time step sizes. We set $m = m + 1$ and begin new predictor corrector iterations for the time interval $[t_m, t_{m+1}]$.

5. Numerical results

We have implemented the splitting scheme (4.1a),(4.1b) along with the predictor corrector continuation strategy (4.3)-(4.18) for two examples showing the isotropic and anisotropic growth of four single crystals. In the first example, four crystals with different orientation angles are initially located around the four corners of the computational domain Ω (cf. Figure 1 below). In the second example, two pairs of crystals with pairwise different orientation angles are initially located inside Ω (cf. Figure 2 below).

The material data, namely the free energy of the low-grain boundaries H (cf. (2.1)), the mobility M_0 (cf. (2.17a)), the mobility related parameter χ (cf. (2.17b)), the amplitude of the anisotropy of the free energy s_0, and the symmetry index m_s (cf. (2.2)) are given in Table 1.

The computational domain has been chosen as the square $\Omega = [0.0\ \mu m, 0.8\ \mu m]^2$. The computational data further include the grid size h (in μm) of the uniform simplicial grid Ω_h with right isosceles, the polynomial degree k of the Lagrangian finite elements, the parameters ε_a and ε_r (cf. (2.2a) and (2.5)), and the data α, ε, ν_{max}, and τ_{min} for the predictor corrector continuation strategy (4.3)-(4.18). These data are given in Table 2.

H	M_0	χ	s_0		m_s	
			Example 1	Example 2	Example 1	Example 2
$1.0 \cdot 10^{-3}$	20.0	0.1	0	0.04	–	4

Table 1. Material data.

h	k	ε_a	ε_r	α	ε	ν_{max}	τ_{min}
$1.29 \cdot 10^{-2}$	2	0.1	$1.0 \cdot 10^{-3}$	1.2	$1.0 \cdot 10^{-3}$	50	$1.0 \cdot 10^{-6}$

Table 2. Computational data.

Example 1: We consider the isotropic growth (i.e., $s_0 = 0$) of four single crystals with different orientation angles. The initial orientation angles Θ_0 and the initial local degree of crystallinity ϕ_0 are given as follows (cf. Figure 1 (top)):

$$\Theta_0 = \begin{cases} 1.2\pi \text{ (dark red) around the right upper corner,} \\ 1.0\pi \text{ (light red) around the right lower corner,} \\ 0.8\pi \text{ (light blue) around the left lower corner,} \\ 0.6\pi \text{ (dark blue) around the left upper corner,} \\ 0.9 \pm 0.05\pi \text{ randomly chosen elsewhere.} \end{cases}$$

$$\phi_0 = \begin{cases} 1.0 \text{ (dark red) around the four corners,} \\ 0.0 \text{ (dark blue) elsewhere.} \end{cases}$$

The four crystals grow along the curvature and start to impinge on each other with the star-shaped area of local degree of crystallinity $\phi = 0$ shrinking (cf. Figure 1 (middle)). This process continues as can be seen in Figure 1 (bottom) which displays the orientation field Θ (bottom left) and the local degree of crystallinity (bottom right) shortly before complete crystallization has settled in.

Example 2: In this example we consider the anisotropic growth ($s_0 = 0.5$) with fourfold symmetry ($m_2 = 4$) of two pairs of crystals with pairwise different orientations initially located inside the computational domain Ω as shown in Figure 2 (top). In particular, the initial orientation angles Θ_0 and the initial local degree of crystallinity ϕ_0 are given as follows:

$$\Theta_0 = \begin{cases} 1.25\pi \text{ (dark red) for the pair of crystals on the right,} \\ 0.75\pi \text{ (dark blue) for the pair of crystals on the left,} \\ 1.0 \pm 0.05\pi \text{ randomly chosen elsewhere.} \end{cases}$$

$$\phi_0 = \begin{cases} 1.0 \text{ (dark red) for the two pairs of crystals,} \\ 0.0 \text{ (dark blue) elsewhere.} \end{cases}$$

We see the crystals grow and impinge attaining a quadratic cross section according to the fourfold symmetry (cf. Figure 2 (middle)). Again, this process continues such that almost at the end of the process there are only two orientations with one narrow grain boundary separating the two orientations (cf. Figure 2 (bottom left)).

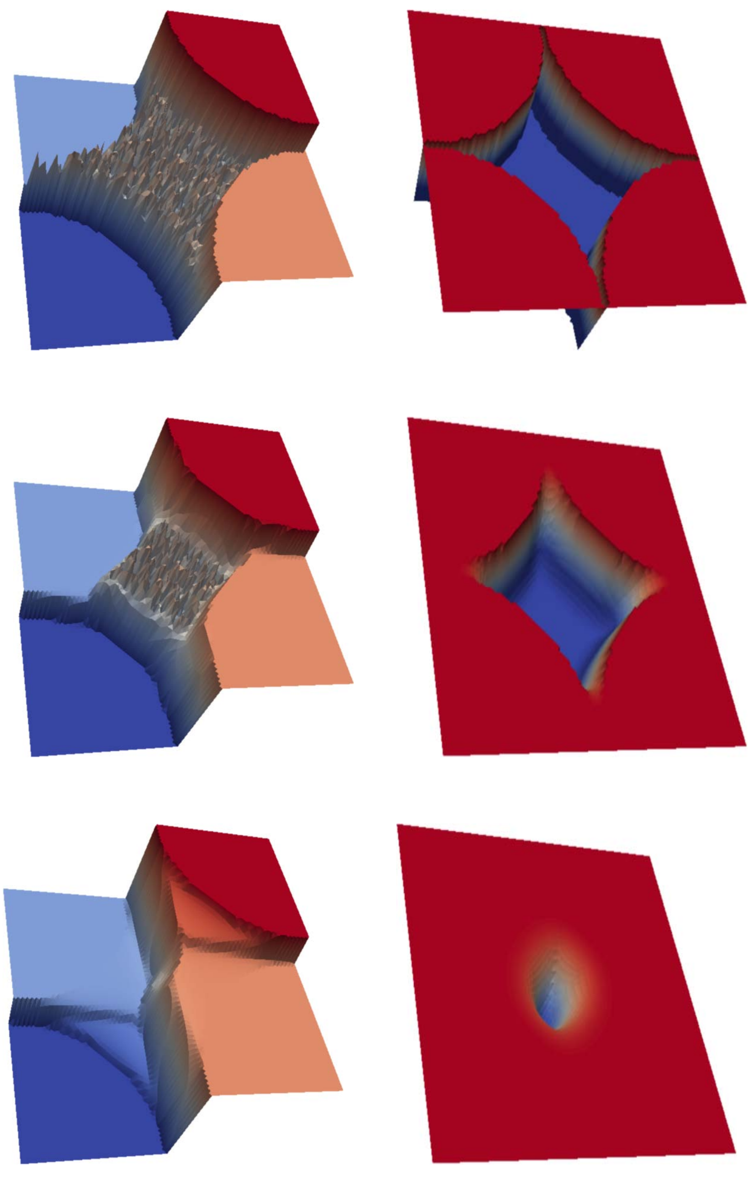

FIGURE 1. Example 1: Isotropic growth of four crystals ($s_0 = 0$) at initial time $t = 0$ sec (top), at time $t = 7.4 \cdot 10^{-2}$ sec (middle), and at final time $t = 9.3{\cdot}10^{-1}$ sec (bottom). Left: Local orientation field Θ. Right: Local degree of crystallinity ϕ.

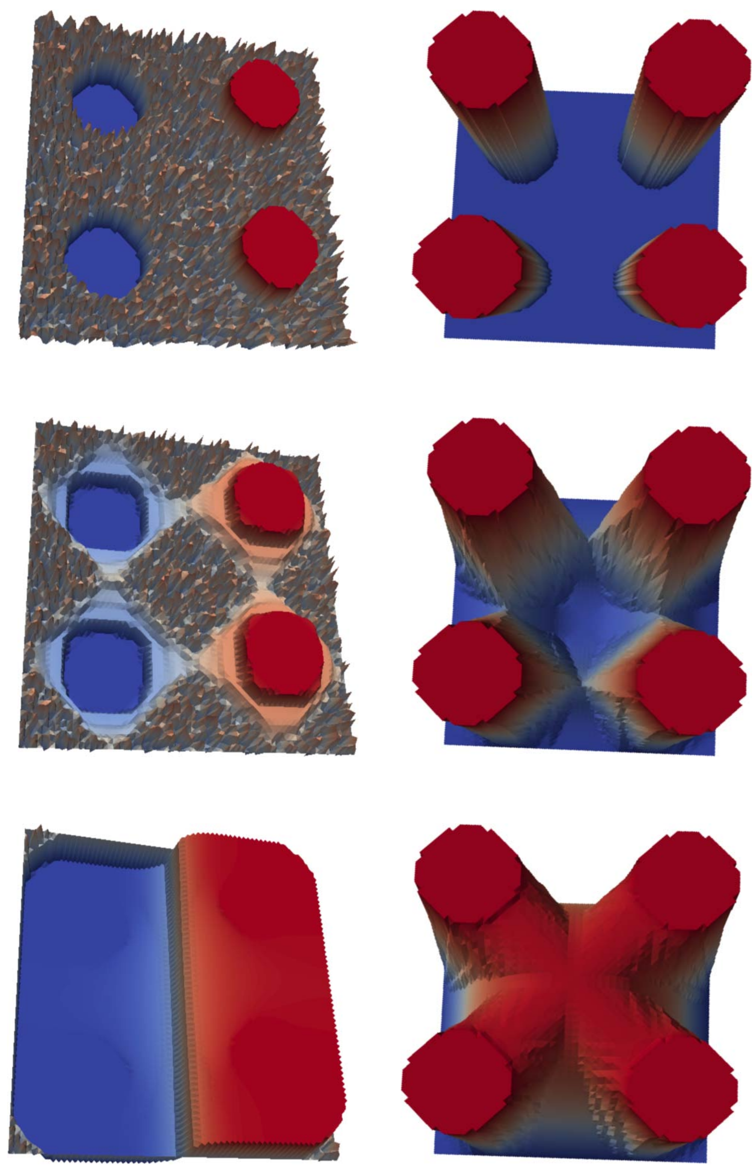

FIGURE 2. Example 2: Crystallization of four crystals with anisotropy ($s_0 = 0.5$,symmetry index $m_s = 4$) at initial time $t = 0$ sec (top), at time $t = 2.40 \cdot 10^{-2}$ sec (middle), and at final time $t = 2.04 \cdot 10^{-1}$ sec (bottom). Left: Local orientation field Θ. Right: Local degree of crystallinity ϕ.

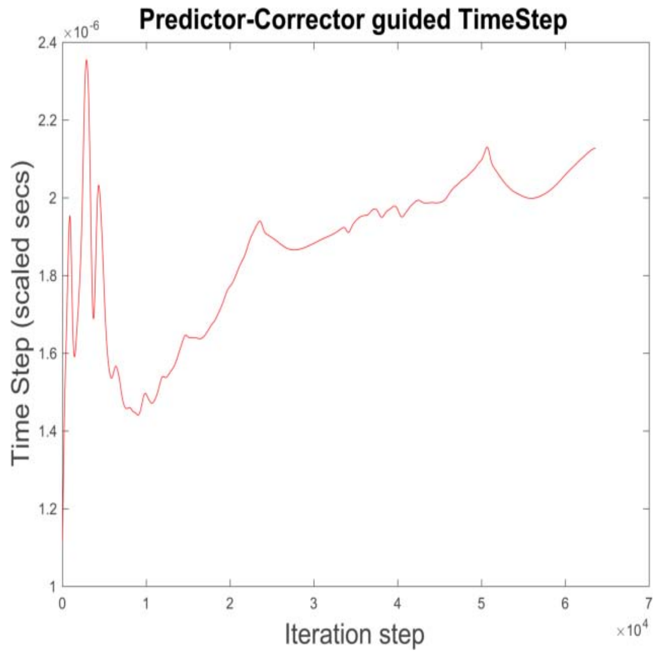

FIGURE 3. Example 2: Performance of the predictor corrector continuation strategy. Adaptive choice of time steps τ_m.

The adaptive choice of the time steps τ_m by means of the predictor corrector continuation strategy (4.3)-(4.18) has been shown to be very beneficial for the numerical solution of the nonlinear systems (4.2a),(4.2b). As expected, the appropriate choice of τ_m is most critical for the fully discrete Θ equation (4.2a), since the original Θ equation (2.14a) represents a very singular diffusion process. As it turned out, both for Example 1 and Example 2 predicted time steps for the fully discrete Θ equation have been frequently rejected and subsequently reduced by the adaptive algorithm, whereas the then predicted time steps for the fully discrete ϕ equation have been always accepted. For Example 2, the adaptive choice of the time steps is displayed in Figure 3.

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