

Rothe's Method for Phase Field Problem

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Abstract In this paper, a phase-field model is considered. Analysis of a time discretization for an initial-boundary value problem for this phase-field model is presented. Convergence is proved and existence, uniqueness and regularity results are derived.

Keywords: Phase-field, phase transitions, semidiscretization.

1. Introduction

Let $\Omega \in \mathbb{R}^n$ ($n \leq 3$) be an open bounded domain with a C^2 boundary and $Q = \Omega \times (0, T)$ the space-time cylinder with lateral surface $S = \partial\Omega \times (0, T)$. We consider the phase field equations (P):

$$\begin{aligned} \frac{\partial \varphi}{\partial t} - \xi^2 \Delta \varphi &= \varphi(\varphi - 1)(1 - 2\varphi) + (\varphi - \varphi^2)F(\theta) && \text{in } Q, \\ \frac{\partial \theta}{\partial t} - \alpha \Delta \theta + v \cdot \nabla \theta &= -\ell \frac{\partial \varphi}{\partial t} && \text{in } Q, \\ \frac{\partial \varphi}{\partial \eta} = 0, \quad \theta &= 0 && \text{on } S, \\ \varphi(x, 0) = \varphi_0(x), \quad \theta(x, 0) &= \theta_0(x) && \text{in } \Omega. \end{aligned}$$

Here, ξ , α , ℓ are positive constants associated to material properties; $v(x, y)$ is a given function weakly solenoidal; $g(s) = s(s - 1)(1 - 2s)$ is the classical double-well potential; θ represents the temperature while φ is the phase field function determining the liquid or solid phase (we refer to [1] for a complete description of the phase-field type model).

As essential tool for the analysis and the numerical treatment of the problem (P) is Rothe's Method (see [5]), which essentially reduces such problem to a boundary value problems of elliptic type. For the stationary phase-field problem we prove an existence result applying Leray-Schauder degree theory (see [2]), compactness arguments and L^p -theory of the elliptic linear equations.

This paper is organized as follows. In the next section, we introduce a time-discretization scheme and state the main results of the paper. Section 2. brings the proof of existence of the discrete solution that is, solution of the corresponding discretized scheme, as well as certain regularity results. Section 3., contains a collection of estimates, uniform with respect to the time-discretization step. In section

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4. we prove existence, uniqueness and regularity of the solution of the problem (P). The solution will be found in the space

$$W_q^{2,1}(Q) = \{u ; u, u_t, D_x u, D_x^2 u \in L^q(Q)\}.$$

More details about the other classical functional spaces will also be used, with standard notations and definitions are given in [5].

Moreover, all along this work we will be using the following technical hypotheses:

(H₀) $\Omega \subset \mathbb{R}^n$, $n = 2$ or 3 , is an open and bounded domain with a C^2 boundary; T is a finite positive number. $Q = \Omega \times (0, T)$ denotes the space-time cylinder with lateral surface $S = \partial\Omega \times (0, T)$.

(H₁) $v(x, t)$ is given function in $L^\infty(0, T; L^2(\Omega)) \cap L^2(0, T; W_2^2(\Omega))$ with $\operatorname{div} v = 0$.

(H₂) $F \in C(\mathbb{R})$ is such that $|F(\cdot)| \leq c_1 < +\infty$.

(H₃) $\varphi_0 \in W_2^{(3/2)+\delta}(\Omega)$ for some $\delta \in (0, 1)$; $\frac{\partial \varphi_0}{\partial \eta} = 0$ on $\partial\Omega$; $\theta_0 \in W_2^1(\Omega)$, where

$$W_q^p(\Omega) = \{u \in L_q(\Omega) ; D^m u \in L_q(Q), |m| \leq p\}$$
 is the usual Sobolev space.

Finally, we remark that, as usual in this kind of context, throughout the article we will denote by c and sometimes c_1, c_2, \dots constants depending only on known quantities.

1.1. Time discretization

We introduce a time-discretization scheme (see [5] p. 241) for the phase-field equations (P).

For any N positive integer, we divide the interval $[0, T]$ into N parts by setting $0 = t_0 < t_1 < \dots < t_m < \dots < t_N = T$ where time-step $\tau = T/N$ and $t_m = m\tau$, $0 \leq m \leq N$. For $m = 1, 2, \dots, N$, we consider the differential-difference equations (PD):

$$\begin{aligned} \delta_t \varphi^m - \xi^2 \Delta \varphi^m &= \varphi^m (\varphi^m - 1) (1 - 2\varphi^m) + (\varphi^m - (\varphi^m)^2) F(\theta^m) & \text{a.e. in } \Omega, \\ \delta_t \theta^m - \alpha \Delta \theta^m + v^m \cdot \nabla \theta^m &= -\ell \delta_t \varphi^m & \text{a.e. in } \Omega, \\ \frac{\partial \varphi^m}{\partial \eta} &= 0, \quad \theta^m = 0 & \text{a.e. on } \partial\Omega, \end{aligned}$$

with given initial values $\varphi^0 = \varphi_0$ and $\theta^0 = \theta_0$.

Here, φ^m , θ^m and v^m , $m = 1, \dots, N$, mean to be approximations of $\varphi(x, t_m)$, $\theta(x, t_m)$ and $v(x, t_m)$, respectively, where $v^m = \frac{1}{\tau} \int_{(m-1)\tau}^{m\tau} v(x, t) dt$. Also, we used the notation

$$\delta_t \varphi^m = (\varphi^m - \varphi^{m-1})/\tau, \quad \delta_t \theta^m = (\theta^m - \theta^{m-1})/\tau,$$

Moreover, we will understand a generalized solution of (PD) in the same as given in [4].

The following existence result for discrete scheme (PD) will be proved in the next section.

Theorem 1.1. *For sufficiently small τ there is a unique generalized solution of the discrete scheme (PD).*

With this result we may introduce the corresponding piecewise constant interpolator functions $\varphi_\tau, \theta_\tau$ and also the corresponding linear interpolator functions $\tilde{\varphi}_\tau, \tilde{\theta}_\tau$:

Definition 1.1. *Consider a partition $\mathcal{P} = \{t_0, t_1, \dots, t_{N-1}, t_N\}$ such that $\tau = T/N$ and $t_m = m\tau, 1 \leq m \leq N$. Then, given $\gamma^m \in L^2(\Omega)$ for $m = 0, \dots, N$, we define the interpolations functions $\gamma_\tau, \tilde{\gamma}_\tau : [0, T] \rightarrow L^2(\Omega)$ as follows: for a.e $x \in \Omega$, and for $t \in [(m-1)\tau, m\tau]$, we set*

$$\gamma_\tau(x, t) = \gamma^m, \quad \tilde{\gamma}_\tau(x, t) = \gamma^m + \left(\frac{t - t_m}{\tau} \right) (\gamma^m - \gamma^{m-1}).$$

In section 4., we will prove the following result

Theorem 1.2. *Assume that $(H_0), (H_1), (H_2)$ and (H_3) holds. Let $\varphi_\tau, \tilde{\varphi}_\tau, \theta_\tau, \tilde{\theta}_\tau$ be functions given by Definition 1.1, and corresponding to the solution of the discrete scheme (PD), obtained in Theorem 1.1. Then, as $\tau \rightarrow 0$, we have the following convergences:*

$$\begin{aligned} \varphi_\tau &\rightharpoonup \varphi & \text{in } L^2(0, T, W_2^2(\Omega)), & \varphi_\tau \overset{*}{\rightharpoonup} \varphi & \text{in } L^\infty(0, T, W_2^1(\Omega)), \\ \theta_\tau &\rightharpoonup \theta & \text{in } L^2(0, T, W_2^1(\Omega)), & \theta_\tau \overset{*}{\rightharpoonup} \theta & \text{in } L^\infty(0, T, L^2(\Omega)), \\ \varphi_\tau &\rightharpoonup \varphi & \text{in } L^4(Q), & \frac{\partial \tilde{\varphi}_\tau}{\partial t} \rightharpoonup \frac{\partial \varphi}{\partial t} & \text{in } L^2(Q) \\ \varphi_\tau &\rightharpoonup \varphi & \text{in } L^2(Q), & & \end{aligned}$$

and the pair (φ, θ) is a unique generalized solution of the problem (P). Moreover, if $\varphi_0 \in W_q^2(\Omega) \cap W_2^{3/2+\delta}(\Omega)$ for some $\delta \in (0, 1)$, and $\theta_0 \in W_q^2(\Omega)$ then this solution satisfies $\varphi \in W_q^{2,1}(Q)$ and $\theta \in W_q^{2,1}(Q)$ with $2 \leq q \leq \infty$.

2. Discrete Solution

Our aim in this section is to prove the existence of solution φ^m, θ^m for a fixed m , assuming that φ^{m-1} and θ^{m-1} are already known. For this, consider the nonlinear system $(P)_1$:

$$-\tau \xi^2 \Delta \varphi + \varphi = \tau \varphi (\varphi - 1)(1 - 2\varphi) + \tau (\varphi - \varphi^2) F(\theta) + f(x) \quad \text{in } \Omega, \quad (2.1)$$

$$-\tau \alpha \Delta \theta + \tau v \cdot \nabla \theta + \theta = -\ell \varphi + g(x) \quad \text{in } \Omega, \quad (2.2)$$

$$\frac{\partial \varphi}{\partial \eta} = 0, \quad \theta = 0 \quad \text{on } \partial \Omega, \quad (2.3)$$

where $(\varphi, \theta) = (\varphi^m, \theta^m)$, $f(x) = \varphi^{m-1}$ and $g(x) = \theta^{m-1} + \ell \varphi^{m-1}$.

We will apply the Leray-Schauder degree theory (see [2]) to prove the solvability of problem $(P)_1$. For this, we reformulate the problem as $T(1, \varphi, \theta) = (\varphi, \theta)$, where $T(\lambda, \cdot)$ is a compact homotopy depending on a parameter $\lambda \in [0, 1]$ defined as follows.

Consider the nonlinear operator

$T : [0, 1] \times W_2^1(\Omega) \times \overset{0}{W}_2^1(\Omega) \rightarrow W_2^1(\Omega) \times \overset{0}{W}_2^1(\Omega)$
 defined as

$$T(\lambda, \phi, \omega) = (\varphi, \theta), \tag{2.4}$$

where (φ, θ) is the unique solution of the following problem $(P_\lambda)_1$:

$$\begin{aligned} -\tau\xi^2\Delta\varphi + \varphi &= \lambda\tau\phi(\phi - 1)(1 - 2\phi) + \lambda\tau(\phi - \phi^2)F(\omega) + \lambda f(x), & \text{in } \Omega, \\ -\tau\alpha\Delta\theta + \tau v \cdot \nabla\theta + \theta &= -\lambda\ell\varphi + \lambda g(x), & \text{in } \Omega, \\ \frac{\partial\varphi}{\partial\eta} &= 0, \quad \theta = 0. & \text{on } \partial\Omega. \end{aligned}$$

To verify that $T(\lambda, \cdot)$ is well defined, we observe that $\phi(\phi - 1)(1 - 2\phi) + (\phi - \phi^2)F(\omega) + f \in L^2(\Omega)$; thus, by the L^p -regularity theory for elliptic linear equations (see [4] Chapter 3), we conclude that the equation $(P_\lambda)_1$ has a unique solution $\varphi \in W_2^2(\Omega) \cap L_0^2(\Omega)$. In addition, $v \in L^4(\Omega)^n$ with $n=2$ or 3 , $\varphi \in L^\infty(\Omega)$ and $g \in L^6(\Omega)$ imply again by L^p -regularity theory for elliptic linear equation that there is a unique solution $\theta \in W_4^2(\Omega)$ for the equation of $(P_\lambda)_1$.

To check the continuity of $T(\lambda, \cdot)$, let $\lambda_n \rightarrow \lambda$ in $[0,1]$ and $(\phi_n, \omega_n) \rightarrow (\phi, \omega)$ in $W_2^1(\Omega) \times \overset{0}{W}_2^1(\Omega)$. Denote $T(\lambda_n, \phi_n, \omega_n) = (\varphi_n^{\lambda_n}, \theta_n^{\lambda_n})$, $T(\lambda, \phi_n, \omega_n) = (\varphi_n^\lambda, \theta_n^\lambda)$ and $T(\lambda, \phi, \omega) = (\varphi^\lambda, \theta^\lambda)$. Thus, from $(\varphi_n^{\lambda_n} - \varphi_n^\lambda, \theta_n^{\lambda_n} - \theta_n^\lambda)$ and L^p -regularity theory for elliptic linear equations, observing that by Sobolev imbedding ($n \leq 3$), $\phi \in W_2^1(\Omega) \subset L^6(\Omega)$ and using the assumptions (H_1) and (H_2) , we obtain the following estimates:

$$\begin{aligned} \|\varphi_n^{\lambda_n} - \varphi_n^\lambda\|_{W_2^1(\Omega)} &\leq c\tau|\lambda_n - \lambda| \left(\|\phi_n\|_{4,\Omega}^2 + (1 + c_1)(\|\phi_n\|_{2,\Omega} + \|\phi_n\|_{6,\Omega}^3) \right) \\ &\quad + c|\lambda_n - \lambda| \|f\|_{2,\Omega}, \end{aligned}$$

$$\|\theta_n^{\lambda_n} - \theta_n^\lambda\|_{W_2^1(\Omega)} \leq c|\lambda_n - \lambda| \left(\|\varphi_n^{\lambda_n}\|_{2,\Omega} + \|g\|_{2,\Omega} \right) + \lambda\ell \|\varphi_n^{\lambda_n} - \varphi_n^\lambda\|_{2,\Omega}.$$

Since the sequence $\{\lambda_n, \phi_n\}$ is bounded in $[0, 1] \times W_2^1(\Omega)$, we conclude that, as $n \rightarrow +\infty$, $\|\varphi_n^{\lambda_n} - \varphi_n^\lambda\|_{W_2^1(\Omega)} \rightarrow 0$ and, consequently $\|\theta_n^{\lambda_n} - \theta_n^\lambda\|_{W_2^1(\Omega)} \rightarrow 0$.

Again, from $(\varphi_n^\lambda - \varphi^\lambda, \theta_n^\lambda - \theta^\lambda)$ as before we have the following estimates:

$$\begin{aligned} \|\varphi_n^\lambda - \varphi^\lambda\|_{W_2^1(\Omega)} &\leq c \left(\|d_n\|_{3,\Omega} \|\phi_n - \phi\|_{6,\Omega} \right) \\ &\quad + \left(\|\phi\|_{3,\Omega} + \|\phi\|_{6,\Omega}^3 \right) \left(\|F(\omega_n) - F(\omega)\|_{6,\Omega} \right), \\ \|\theta_n^\lambda - \theta^\lambda\|_{W_2^1(\Omega)} &\leq c \left(\|\varphi_n^\lambda - \varphi^\lambda\|_{2,\Omega} \right). \end{aligned}$$

where $d_n = 3\tau(\phi_n + \phi) - 2\tau(\phi_n^2 + \phi_n\phi + \phi^2) - \tau + \tau F(\omega_n)(1 - \phi_n - \phi) \in L^3(\Omega)$.

Using the assumption (H_2) and $(\phi_n, \omega_n) \rightarrow (\phi, \omega)$ in $W_2^1(\Omega) \times \overset{0}{W}_2^1(\Omega)$, we get $\|\varphi_n^\lambda - \varphi^\lambda\|_{W_2^1(\Omega)} \rightarrow 0$ as $n \rightarrow +\infty$. Consequently, $\|\theta_n^\lambda - \theta^\lambda\|_{W_2^1(\Omega)} \rightarrow 0$ as $n \rightarrow +\infty$, and we obtain the continuity of T .

The mapping T given by (2.4) is also compact. In fact, if $\{(\lambda_n, \phi_n, \omega_n)\}$ is any bounded sequence in $[0, 1] \times W_2^1(\Omega) \times \overset{0}{W}_2^1(\Omega)$, the previous arguments can be applied

to obtain exactly the same sort of estimates for $T(\lambda_n, \phi_n, \omega_n) = (\varphi_n, \theta_n)$. These estimates imply that $\|\varphi_n\|_{W_2^1(\Omega)} \leq c$ and $\|\theta_n\|_{W_2^1(\Omega)} \leq c$.

Applying again the L^p -regularity theory for elliptic equations, we obtain, for all n , that $\|\varphi_n\|_{W_2^2(\Omega)} \leq c$ and $\|\theta_n\|_{W_2^2(\Omega)} \leq c$. These estimates show that the norms of the elements of the sequence $\{T(\lambda_n, \phi_n, \omega_n)\} = \{(\varphi_n, \theta_n)\}$ are uniformly bounded with respect to n in the functional space $W_2^2(\Omega) \times W_2^2(\Omega)$. Since the imbedding of $W_2^2(\Omega) \times (W_2^2(\Omega) \cap \overset{0}{W}_2^1(\Omega))$ into $W_2^1(\Omega) \times \overset{0}{W}_2^1(\Omega)$ is compact, there exists a subsequence of $T(\lambda_n, \phi_n, \omega_n)$ converging in $W_2^1(\Omega) \times \overset{0}{W}_2^1(\Omega)$ and the compactness of T is proved.

In the following, we will show that any possible fixed point of $T(\lambda, \cdot)$ can be estimated independently of $\lambda \in [0, 1]$, that is, we will show that if $(\varphi, \theta) \in W_2^1(\Omega) \times \overset{0}{W}_2^1(\Omega)$ is such that $T(\lambda, \varphi, \theta) = (\varphi, \theta)$, for some $\lambda \in [0, 1]$, then there exists a constant $\beta > 0$ such that

$$\|(\varphi, \theta)\|_{W_2^1(\Omega) \times W_2^1(\Omega)} < \beta. \tag{2.5}$$

For this, we recall that such fixed point $(\varphi, \theta) \in W_2^1(\Omega) \times \overset{0}{W}_2^1(\Omega)$ solves the problem $(P_\lambda)_2$:

$$\begin{aligned} -\tau\xi^2\Delta\varphi + \varphi &= \lambda\tau\varphi(\varphi - 1)(1 - 2\varphi) + \lambda\tau(\varphi - \varphi^2)F(\theta) + \lambda f(x) & \text{in } \Omega, \\ -\tau\alpha\Delta\theta + \tau v \cdot \nabla\theta + \theta &= \lambda\ell\varphi + \lambda g(x) & \text{in } \Omega, \\ \frac{\partial\varphi}{\partial\eta} &= 0, \quad \theta = 0 & \text{on } \partial\Omega. \end{aligned}$$

If we multiply these differential equations by φ and θ , respectively, integrate by parts and use Young's inequality we obtain in the usual manner the following estimates:

$$\begin{aligned} \tau\xi^2 \int_{\Omega} |\nabla\varphi|^2 dx + \frac{1}{2} \int_{\Omega} |\varphi|^2 dx + \frac{\lambda\tau}{2} \int_{\Omega} |\varphi|^4 dx &\leq \tau c_2 \|\varphi\|_{2,\Omega}^2 + c_3 \|f\|_{2,\Omega}^2, \\ \tau\alpha \int_{\Omega} |\nabla\theta|^2 dx + \frac{1}{4} \int_{\Omega} |\theta|^2 dx &\leq c_4 \left(\|\varphi\|_{2,\Omega}^2 + \|g\|_{2,\Omega}^2 \right). \end{aligned}$$

Here we also used the assumption (H_2) and that $\max_{s \in \mathbb{R}} (3s - s^2 - 1)$ is finite.

Thus, by taking $\tau < 1/2c_2$, we conclude that $\|\varphi\|_{W_2^1(\Omega)} \leq c \|f\|_{2,\Omega}$ and, consequently $\|\theta\|_{W_2^1(\Omega)} \leq c \left(\|f\|_{2,\Omega} + \|g\|_{2,\Omega} \right)$, where c depends on $\Omega, \ell, \xi, \alpha, \tau \|F\|_\infty$ and $\max_{s \in \mathbb{R}} (3s - s^2 - 1)$.

Thus, to obtain the stated result, it is enough to take any constant $\beta > \max \left\{ c \|f\|_{2,\Omega}, c \left(\|f\|_{2,\Omega} + \|g\|_{2,\Omega} \right) \right\}$. By denoting

$$B_\beta = \left\{ (\varphi, \theta) \in W_2^1(\Omega) \times \overset{0}{W}_2^1(\Omega) ; \|(\varphi, \theta)\|_{W_2^1(\Omega) \times W_2^1(\Omega)} < \beta \right\}$$

(2.5) ensures in particular that $T(\lambda, \varphi, \theta) \neq (\varphi, \theta), \forall (\varphi, \theta) \in \partial B_\beta, \forall \lambda \in [0, 1]$.

According to property above and the compactness of $T(\lambda, \cdot)$, we may consider the Leray-Schauder degree $D(Id - T(\lambda, \cdot), B_\beta, 0)$, $\forall \lambda \in [0, 1]$ (see Deimling [2]). The homotopy invariance of the degree implies

$$D(Id - T(0, \cdot), B_\beta, 0) = D(Id - T(1, \cdot), B_\beta, 0). \tag{2.6}$$

Now, by choosing $\beta > 0$ large enough so that the ball B_β contains the unique solution of the equation $T(0, \varphi, \theta) = (\varphi, \theta)$. Therefore $D(Id - T(0, \cdot), B_\beta, 0) = 1$, and from (2.6) we conclude that problem $(P)_1$ has a solution $(\varphi, \theta) \in W_2^1(\Omega) \times \overset{0}{W}_2^1(\Omega)$.

Using the assumption (H_2) and L^p -regularity theory for elliptic linear equations it is easy to conclude that $\varphi \in W_2^2(\Omega) \cap C^{1,\sigma}(\overline{\Omega})$ with $\sigma = 1 - n/4$. Now, applying the L^p -regularity theory for elliptic linear equations in (2.2) with $v \in L^4(\Omega)^n$, $\varphi \in L^2(\Omega)$ and $g \in L^2(\Omega)$, we obtain $\theta \in W_2^2(\Omega) \cap C^{1,\sigma}(\overline{\Omega})$ with $\sigma = 1 - n/4$.

Moreover, using a standard contradiction argument, we can prove the uniqueness of solutions of problem $(P)_1$ for sufficiently small τ , completing the proof the Theorem 1.1

3. A Priori Estimates

In this section we will be interested in obtaining *a priori* estimates, which are uniform with respect to τ . For this, if we multiply the first equation of problem (PD) by $\delta_t \varphi^m$, φ^m and $-\Delta \varphi^m$, respectively, integrate by parts, we obtain in the usual manner the following estimates:

$$\begin{aligned} & \int_{\Omega} (\delta_t \varphi^m)^2 dx + \frac{\xi^2}{\tau} \int_{\Omega} \nabla \varphi^m (\nabla \varphi^m - \nabla \varphi^{m-1}) dx + \frac{2}{\tau} \int_{\Omega} (\varphi^m)^4 dx \\ & \leq 3 \int_{\Omega} |\varphi^m|^2 |\delta_t \varphi^m| dx + \int_{\Omega} |\varphi^m| |\delta_t \varphi^m| dx + \frac{2}{\tau} \int_{\Omega} |\varphi^m|^3 |\varphi^{m-1}| dx \\ & + \int_{\Omega} |F(\theta^m)| |\varphi^m| |\delta_t \varphi^m| dx + \int_{\Omega} |\varphi^m|^2 |F(\theta^m)| |\delta_t \varphi^m| dx, \\ & \frac{1}{\tau} \int_{\Omega} (\varphi^m - \varphi^{m-1}) \varphi^m dx + \xi^2 \int_{\Omega} |\nabla \varphi^m|^2 dx + \int_{\Omega} (\varphi^m)^4 dx \\ & \leq \int_{\Omega} (3\varphi^m - 1 - (\varphi^m)^2) (\varphi^m)^2 dx + \int_{\Omega} |F(\theta^m)| |\varphi^m|^2 dx + \int_{\Omega} |\varphi^m|^2 |F(\theta^m)| |\varphi^m| dx, \\ & \xi^2 \int_{\Omega} |\Delta \varphi^m| dx + 9 \int_{\Omega} |\nabla \varphi^m|^2 (\varphi^m)^2 dx \leq \int_{\Omega} |\varphi^m| |\Delta \varphi^m| dx + \int_{\Omega} |\varphi^m|^2 |\Delta \varphi^m| dx \\ & + \int_{\Omega} |\varphi^m| |F(\theta^m)| |\Delta \varphi^m| dx + \int_{\Omega} |\varphi^m|^2 |F(\theta^m)| |\Delta \varphi^m| dx + \int_{\Omega} |\delta_t \varphi^m| |\Delta \varphi^m| dx. \end{aligned}$$

Using the assumption (H_2) with $\max_{s \in \mathbb{R}, x \in \Omega} (3s - 1 - s^2)$ is finite, Hölder's, Young's and Poincaré inequalities, and applying the following relation

$$2 \int_{\Omega} \chi(\chi - \psi) dx = \int_{\Omega} |\chi|^2 dx - \int_{\Omega} |\psi|^2 dx + \int_{\Omega} |\chi - \psi|^2 dx, \tag{3.1}$$

we find

$$\begin{aligned} & \tau \|\delta_t \varphi^m\|_{2,\Omega}^2 + \frac{1}{\tau} \left(\|\nabla \varphi^m\|_{2,\Omega}^2 - \|\nabla \varphi^{m-1}\|_{2,\Omega}^2 + \|\nabla \varphi^m - \nabla \varphi^{m-1}\|_{2,\Omega}^2 \right) \\ & + \frac{1}{2\tau} \left(\|\varphi^m\|_{4,\Omega}^4 - \|\varphi^{m-1}\|_{4,\Omega}^4 \right) \leq c_2 \|\varphi^m\|_{4,\Omega}^4 + c \|\varphi^m\|_{2,\Omega}^2, \end{aligned} \quad (3.2)$$

$$\begin{aligned} & \frac{1}{\tau} \left(\|\varphi^m\|_{2,\Omega}^2 - \|\varphi^{m-1}\|_{2,\Omega}^2 + \|\varphi^m - \varphi^{m-1}\|_{2,\Omega}^2 \right) + \xi^2 \|\nabla \varphi^m\|_{2,\Omega}^2 + \frac{1}{2} \|\varphi^m\|_{4,\Omega}^4 \\ & \leq c \|\varphi^m\|_{2,\Omega}^2, \end{aligned} \quad (3.3)$$

$$\tau \|\Delta \varphi^m\|_{2,\Omega}^2 \leq c\tau \left(\|\nabla \varphi^m\|_{2,\Omega}^2 + \|\varphi^m\|_{4,\Omega}^4 + \|\delta_t \varphi^m\|_{2,\Omega}^2 \right). \quad (3.4)$$

By multiplying (3.3) by $4c_2$ and adding the result to estimate (3.2), we get

$$\begin{aligned} & \frac{1}{\tau} \left(\|\varphi^m\|_{2,\Omega}^2 - \|\varphi^{m-1}\|_{2,\Omega}^2 + \|\varphi^m - \varphi^{m-1}\|_{2,\Omega}^2 \right) \\ & + \frac{1}{\tau} \left(\|\nabla \varphi^m\|_{2,\Omega}^2 - \|\nabla \varphi^{m-1}\|_{2,\Omega}^2 + \|\nabla \varphi^m - \nabla \varphi^{m-1}\|_{2,\Omega}^2 \right) \\ & + \|\nabla \varphi^m\|_{2,\Omega}^2 + \|\varphi^m\|_{4,\Omega}^4 + \|\delta_t \varphi^m\|_{2,\Omega}^2 + \frac{1}{2\tau} \left(\|\varphi^m\|_{4,\Omega}^4 - \|\varphi^{m-1}\|_{4,\Omega}^4 \right) \\ & \leq c \|\varphi^m\|_{2,\Omega}^2. \end{aligned}$$

By adding these relations and (3.4) for $m = 1, 2, \dots, r$, with $1 \leq r \leq N$, we finally get

$$\begin{aligned} & \|\varphi^r\|_{W_2^1(\Omega)}^2 + \|\varphi^r\|_{4,\Omega}^4 + \sum_{m=1}^r \|\varphi^m - \varphi^{m-1}\|_{W_2^1(\Omega)}^2 + \tau \sum_{m=1}^r \|\nabla \varphi^m\|_{2,\Omega}^2 \\ & + \tau \sum_{m=1}^r \|\varphi^m\|_{4,\Omega}^4 + \tau \sum_{m=1}^r \|\delta_t \varphi^m\|_{2,\Omega}^2 \leq c \|\varphi_0\|_{W_2^1(\Omega)}^2 + c\tau \sum_{m=1}^r \|\varphi^m\|_{2,\Omega}^2, \\ & \tau \sum_{m=1}^r \|\Delta \varphi^m\|_{2,\Omega}^2 \leq c \left(\tau \sum_{m=1}^r \|\nabla \varphi^m\|_{2,\Omega}^2 + \tau \sum_{m=1}^r \|\varphi^m\|_{4,\Omega}^4 + \tau \sum_{m=1}^r \|\delta_t \varphi^m\|_{2,\Omega}^2 \right). \end{aligned}$$

Now, we apply Gronwall's lemma in a discrete form (see for instance [7] p.413) to conclude that

$$\|\varphi^r\|_{W_2^1(\Omega)} \leq c \|\varphi_0\|_{W_2^1(\Omega)} \quad \text{for } r = 0, 1, \dots, N. \quad (3.5)$$

By going back to (3.5), we obtain the following estimates:

$$\max_{1 \leq r \leq N} \|\varphi^r\|_{W_2^1(\Omega)}^2 \leq c, \quad \tau \sum_{m=1}^r \|\nabla \varphi^m\|_{2,\Omega}^2 \leq c, \quad (3.6)$$

$$\sum_{m=1}^r \|\varphi^m - \varphi^{m-1}\|_{W_2^1(\Omega)}^2 \leq c, \quad \tau \sum_{m=1}^r \|\varphi^m\|_{4,\Omega}^4 \leq c, \quad (3.7)$$

$$\tau \sum_{m=1}^r \|\delta_t \varphi^m\|_{2,\Omega}^2 \leq c, \quad \tau \sum_{m=1}^r \|\Delta \varphi^m\|_{2,\Omega}^2 \leq c. \quad (3.8)$$

Now, by multiplying the second equation of (PD) by θ^m , integrating over Ω , using Green's formula and relation (3.1) together with Young's inequality, we get

$$\begin{aligned} & \frac{1}{2\tau} \left(\|\theta^m\|_{2,\Omega}^2 - \|\theta^{m-1}\|_{2,\Omega}^2 + \|\theta^m - \theta^{m-1}\|_{2,\Omega}^2 \right) + \alpha \|\nabla \theta^m\|_{2,\Omega}^2 \\ & \leq \frac{\ell^2}{2} \|\delta_t \varphi^m\|_{2,\Omega}^2 + \frac{1}{2} \|\theta^m\|_{2,\Omega}^2. \end{aligned}$$

By adding these relations for $m = 1, 2, \dots, r$, with $1 \leq r \leq N$ and by combining the result with estimate (3.8) and again applying Gronwall's lemma in a discrete form we conclude that

$$\|\theta^r\|_{2,\Omega} \leq C \left(\|\theta_0\|_{2,\Omega} + \|\varphi_0\|_{2,\Omega} \right) \text{ for } r = 0, 1, \dots, N.$$

We can treat this expression as we did before to obtain the following estimates:

$$\max_{1 \leq r \leq N} \|\theta^r\|_{2,\Omega}^2 \leq c, \quad \tau \sum_{m=1}^r \|\nabla \theta^m\|_{2,\Omega}^2 \leq c, \quad \sum_{m=1}^r \|\theta^m - \theta^{m-1}\|_{2,\Omega}^2 \leq c. \quad (3.9)$$

4. Proof of Theorem 1.2

We start by observing that with the notations of Definition 1.1, we may rewrite the scheme (P) in terms of $\varphi_\tau, \tilde{\varphi}_\tau, \theta_\tau, \tilde{\theta}_\tau$ as follows.

$$\frac{\partial \tilde{\varphi}_\tau}{\partial t} - \xi^2 \Delta \varphi_\tau = \varphi_\tau (\varphi_\tau - 1) (1 - 2\varphi_\tau) + (\varphi_\tau - \varphi_\tau^2) F(\theta_\tau) \quad \text{in } Q, \quad (4.1)$$

$$\frac{\partial \tilde{\theta}_\tau}{\partial t} - \alpha \Delta \theta_\tau + v_\tau \cdot \nabla \theta_\tau = -\ell \frac{\partial \tilde{\varphi}_\tau}{\partial t} \quad \text{in } Q, \quad (4.2)$$

$$\frac{\partial \varphi_\tau}{\partial \eta} = 0, \quad \theta_\tau = 0 \quad \text{on } S, \quad (4.3)$$

$$\tilde{\varphi}_\tau(x, 0) = \varphi_0(x), \quad \tilde{\theta}_\tau(x, 0) = \theta_0(x) \quad \text{in } \Omega. \quad (4.4)$$

Here v_τ denotes the interpolation function as in Definition 1.1.

By rewriting the estimates obtained in the last section in terms of the interpolations functions $\varphi_\tau, \tilde{\varphi}_\tau, \theta_\tau, \tilde{\theta}_\tau$, we obtain

Lemma 4.1.

$$\|\varphi_\tau\|_{L^\infty(0,T;W_2^1(\Omega))} + \|\tilde{\varphi}_\tau\|_{L^\infty(0,T;W_2^1(\Omega))} + \|\varphi_\tau\|_{W_2^{2,0}(Q)} + \|\tilde{\varphi}_\tau\|_{W_2^{2,0}(Q)} \leq c,$$

$$\|\theta_\tau\|_{L^\infty(0,T;W_2^1(\Omega))} + \|\tilde{\theta}_\tau\|_{W_2^{1,0}(Q)} \leq c,$$

$$\|\varphi_\tau\|_{4,Q} + \left\| \frac{\partial \tilde{\varphi}_\tau}{\partial t} \right\|_{2,Q} \leq c,$$

where $W_2^{2,0}(Q) = L^2(0, T, W_2^2(\Omega))$.

Proof. From (3.6)-(3.8), we obtain

$$\left\| \frac{\partial \tilde{\varphi}_\tau}{\partial t} \right\|_{2,Q}^2 = \sum_{m=1}^N \int_{(m-1)\tau}^{m\tau} \|\delta_t \varphi^m\|_{2,\Omega}^2 dt \leq \tau \sum_{m=1}^N \|\delta_t \varphi^m\|_{2,\Omega}^2 \leq c.$$

$$\|\nabla\varphi_\tau\|_{2,Q}^2 = \sum_{m=1}^N \int_{(m-1)\tau}^{m\tau} \|\nabla\varphi^m\|_{2,\Omega}^2 dt \leq \tau \sum_{m=1}^N \|\nabla\varphi^m\|_{2,\Omega}^2 \leq c.$$

By similar arguments, using estimates (3.6)-(3.8) and (3.9), we obtain the other estimates of the statement. \square

Now, by using the estimates from Lemma 4.1, there exist subsequences, which for simplicity we still denote $\varphi_\tau, \theta_\tau, \tilde{\varphi}_\tau, \tilde{\theta}_\tau$, such that as $\tau \rightarrow 0$ they satisfy

$$\varphi_\tau \rightharpoonup \varphi \text{ in } L^2(0, T, W_2^2(\Omega)), \quad \varphi_\tau \overset{*}{\rightharpoonup} \varphi \text{ in } L^\infty(0, T, W_2^1(\Omega)), \tag{4.5}$$

$$\theta_\tau \rightharpoonup \theta \text{ in } L^2(0, T, W_2^1(\Omega)), \quad \theta_\tau \overset{*}{\rightharpoonup} \theta \text{ in } L^\infty(0, T, L^2(\Omega)), \tag{4.6}$$

$$\tilde{\varphi}_\tau \rightharpoonup \tilde{\varphi} \text{ in } L^2(0, T, W_2^1(\Omega)), \quad \varphi_\tau \rightarrow \varphi \text{ in } L^4(Q), \tag{4.7}$$

$$\tilde{\theta}_\tau \rightharpoonup \tilde{\theta} \text{ in } L^2(0, T, W_2^1(\Omega)), \quad \frac{\partial \tilde{\varphi}_\tau}{\partial t} \rightharpoonup \frac{\partial \tilde{\varphi}}{\partial t} \text{ in } L^2(Q). \tag{4.8}$$

We must control the differences $\tilde{\varphi}_\tau - \varphi_\tau$ with respect to suitable norms. From their definitions,

$$\|\tilde{\varphi}_\tau - \varphi_\tau\|_{2,Q}^2 = \sum_{m=1}^N \int_{(m-1)\tau}^{m\tau} (t - t_m)^2 \|\delta_t \varphi^m\|_{2,\Omega}^2 = \frac{\tau^2}{3} \left(\tau \sum_{m=1}^N \|\delta_t \varphi^m\|_{2,\Omega}^2 \right).$$

Therefore, from (3.8), we conclude that $\|\tilde{\varphi}_\tau - \varphi_\tau\|_{L^2(Q)} \leq c\tau$. Thus, from (4.5) and (4.7), we obtain $\varphi = \tilde{\varphi}$, *a.e.* in Q . This, (4.5) and (4.7) in particular imply $\tilde{\varphi}_\tau \rightharpoonup \varphi$ in $L^2(0, T; W_2^1(\Omega))$.

Using (4.8) and the Aubin-Lions Compactness Lemma (see [8], for instance,) we derive also the strong convergence $\varphi_\tau \rightarrow \varphi$ in $L^2(Q)$.

Now we are ready to pass to the limit in scheme (4.1), (4.2), (4.3), (4.4) and to verify that (φ, θ) is in fact a generalized solution in the same sense as given in [5, p. 26].

For this, we take ϕ and ψ in $C^1(Q)$ such that $\phi(\cdot, T) = \psi(\cdot, T) = 0$. We use them to multiply the suitable equations and integrate over Q . Due to the kind of convergences we have already established, passing to the limit in these terms are rather standard. So, we briefly describe the process for the nonlinear terms. For instance, by using the strong convergence, we obtain

$$\int_Q \varphi_\tau(\varphi_\tau - 1)(1 - 2\varphi_\tau) \phi \, dx \, dt \rightarrow \int_Q \varphi(\varphi - 1)(1 - 2\varphi) \phi \, dx \, dt.$$

Consider $h_\tau = |F(\theta_\tau) - F(\theta)|^6$. Since $F(y)$ is continuous and (4.6) is valid, passing to a subsequence if necessary, we know that $h_\tau \rightarrow 0$ almost everywhere in Q . Also, $|h_\tau| \leq \|F(\theta)\|_\infty^6$ *a.e.* and therefore $h_\tau \rightarrow 0$ in $L^1(Q)$ by Lebesgue dominated convergence theorem. Thus, $F(\theta_\tau) \rightarrow F(\theta)$ in $L^6(Q)$, what together with (4.7) implies

$$\int_Q (\varphi_\tau - \varphi_\tau^2) F(\theta_\tau) \phi \, dx \, dt \rightarrow \int_Q (\varphi - \varphi^2) F(\theta) \phi \, dx \, dt$$

Also, it is easily show that $v_\tau \rightarrow v$ in $L^4(Q)$ (see [6]), by using this convergence, the fact that $\text{div } v = 0$ and (4.6), we can pass to the limit as $\tau \rightarrow 0$ in (4.1), (4.2), (4.3), (4.4) and conclude that (φ, θ) is a generalized solution of (P).

By a bootstrap argument, an interpolation argument (see [5] p.466) and applying L^p -theory of parabolic linear equations (see [5] p.351), recalling the given smoothness of (φ_0, θ_0) we conclude that $(\varphi, \theta) \in W_q^{2,1}(Q) \times W_q^{2,1}(Q)$ with $2 \leq q \leq \infty$.

Moreover, by using the same arguments of [3], we can be prove uniqueness of solutions of problem (P), completing the proof of Theorem 1.2.

References

- [1] C. Beckermann, H.J. Diepers, I. Steinbach, A. Karma, X. Tong, Modeling melt convection in phase-field simulations of solidification, *J. Comp. Phys.*, **154** (1999), 468-496.
- [2] K. Deimling, "Nonlinear Functional Analysis", Springer-Verlag, 1984.
- [3] K.H. Hoffman, L. Jiang, Optimal control a phase field model for solidification, *Numer. Funct. Anal. Optimiz.* **13**, No. 1-2 (1992), 11-27.
- [4] O.A. Ladyzenskaja, N.N. Ural'ceva, "Linear and Quasilinear Elliptic Equations", Academic Press, 1968.
- [5] O.A. Ladyzenskaja, V.A. Solonnikov, N.N. Ural'ceva, "Linear and Quasilinear Equations of Parabolic Type", American Mathematical Society, Providence, 1968.
- [6] M. Marion, R. Temam, "Navier-Stokes Equations: Theory and Approximation", Handbook of Numerical Analysis, Vol VI, 1998.
- [7] J.T. Oden, J.N. Reddy, "An Introduction to the Mathematical Theory of Finite Element", John Wiley & Sons, 1976.
- [8] J. Simon, Compact sets in the space $L^p(0, T; B)$. *Annali di Matematica Pura ed Applicata*, Serie Quarta, Tomo CXLVI, 1987, pp. 65-96.