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Fractional Steps Scheme to Approximate the Phase Field Transition System Endowed with Inhomogeneous/Homogeneous Cauchy-Neumann/Neumann Boundary Conditions

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Abstract: Here, we consider the phase field transition system (a nonlinear system of parabolic type) introduced by Caginalp to distinguish between the phases of the material that are involved in the solidification process. We start by investigating the solvability of such boundary value problems in the class $W_p^{1,2}(Q) \times W_\nu^{1,2}(Q)$. One proves the existence, the regularity, and the uniqueness of solutions, in the presence of the cubic nonlinearity type. On the basis of the convergence of an iterative scheme of the fractional steps type, a conceptual numerical algorithm, **alg-frac_sec-ord-varphi_PHT**, is elaborated in order to approximate the solution of the nonlinear parabolic problem. The advantage of such an approach is that the new method simplifies the numerical computations due to its decoupling feature. An example of the numerical implementation of the principal step in the conceptual algorithm is also reported. Some conclusions are given are also given as new directions to extend the results and methods presented in the present paper.

Keywords: boundary value problems for nonlinear parabolic PDE; fractional steps method; convergence of numerical scheme; numerical algorithm; phase-changes

MSC: 35K55; 65N06; 65N12; 80Axx

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1. Introduction

On a bounded domain $\Omega \subset \mathbb{R}^n$, $n \in \{1,2,3\}$, with a C^2 boundary $\partial\Omega$ and for a finite time $T > 0$, we consider the following nonlinear second-order parabolic system with respect to the unknown functions $u(t,x)$ and $\varphi(t,x)$:

$$\begin{cases} p_1 \dfrac{\partial}{\partial t} u(t,x) + q_1 \dfrac{\partial}{\partial t}\varphi(t,x) - p_2 \Delta u(t,x) = p_3 g_1(t,x) \\ q_2 \dfrac{\partial}{\partial t}\varphi(t,x) - q_3 \operatorname{div}\Big(K\big(t,x,\varphi(t,x)\big)\,\nabla\varphi(t,x)\Big) \\ \qquad\qquad = q_4\left[\varphi(t,x) - \varphi^3(t,x)\right] + p_4 u(t,x) + q_5 g_2(t,x) \end{cases} \quad \text{in } Q, \tag{1}$$

where:

- $Q := (0,T] \times \Omega$;
- $u(t,x)$—represents the *reduced temperature distribution* in Q, i.e., $u(t,x) = \theta(t,x) - \theta_M$, with $\theta(t,x)$ representing the temperature of the material at $(t,x) \in Q$ and θ_M representing *the melting temperature* (the temperature at which solid and liquid may co-exist in equilibrium, separated by a planar interface—see ([1], Figure 1.1, p. 31));

- $\varphi(t,x)$—is the *phase function* (the order parameter—as can be seen in ([1], Figure 1.2, p. 35)) which is used to distinguish between the states (phases) of the material which occupy the region Ω at every time $t \in [0,T]$;
- $\dfrac{\partial}{\partial s}u(s,\cdot)$ (u_s in short) is the partial derivative of $u(s,\cdot)$ relative to $s \in (0,T]$;
- $p_1, p_2, p_3, p_4, q_1, q_2, q_3, q_4$ and q_5 are positive values;
- p, q are given numbers which satisfy

$$q \geq p \geq 2; \tag{2}$$

- $K(s,y,\varphi(s,y))$—is the mobility function (attached to the solution $\varphi(s,y)$, $(s,y) \in Q$, of $(1)_2$) (see [2,3] for more details);
- $g_1(t,x) \in L^p(Q)$, $g_2(t,x) \in L^q(Q)$ are given functions (can be also interpreted as *distributed controls*). Let us remark that, according to (2), the term $g_1(t,x)$ in $(1)_1$ could have weaker regularity properties than $g_2(t,x)$ in $(1)_2$ (see [1–11]).

Together with (1), we consider the non-homogeneous Cauchy–Neumann boundary condition (unknown functions $u(t,x)$) and homogeneous Neumann boundary condition (unknown functions $\varphi(t,x)$):

$$\begin{cases} p_2\dfrac{\partial}{\partial \mathbf{n}}u(t,x) + p_5 u(t,x) = g_{fr}(t,x) \\ q_3\dfrac{\partial}{\partial \mathbf{n}}\varphi(t,x) = 0 \end{cases} \quad \text{on } \Sigma, \tag{3}$$

and initial conditions

$$\begin{cases} u(0,x) = u_0(x) \\ \varphi(0,x) = \varphi_0(x) \end{cases} \quad \text{on } \Omega, \tag{4}$$

where $\Sigma = (0,T] \times \partial\Omega$, and:

- $p_5 > 0$ is a physical parameter representing the *heat transfer coefficient*;
- $g_{fr}(t,x) \in W_p^{1-\frac{1}{2p},2-\frac{1}{p}}(\Sigma)$, $p \geq 2$—is a given function: the temperature of the surrounding at $\partial\Omega$ for each time $t \in [0,T]$ (can also be interpreted as *boundary control*);
- $u_0, \varphi_0 \in W_p^{2-\frac{2}{p}}(\Omega)$, with $p_2\frac{\partial}{\partial \nu}u_0 + p_5 u_0 = g_{fr}(0,x)$ and $q_3\frac{\partial}{\partial \nu}\varphi_0 = 0$;
- $\mathbf{n} = \mathbf{n}(x)$ has the same meaning as in [1,2,10–13].

2. Well-Posedness of Solutions to the Nonlinear Second-Order System (1) + (3) + (4)

Following the same reasoning as in Miranville and Moroşanu [1], the phase-field transition system (1) + (3) + (4) can be written suitably in the following form

$$\begin{cases} p_1\dfrac{\partial}{\partial t}u(t,x) - p_2\Delta u(t,x) = -q_1\dfrac{\partial}{\partial t}\varphi(t,x) + p_3 g_1(t,x) & \text{in } Q \\ p_2\dfrac{\partial}{\partial \mathbf{n}}u(t,x) + p_5 u(t,x) = g_{fr}(t,x) & \text{in } \Sigma \\ u(0,x) = u_0(x) & \text{on } \Omega, \end{cases} \tag{5}$$

$$\begin{cases} q_2\dfrac{\partial}{\partial t}\varphi(t,x) - q_3\mathrm{div}\Big(K\big(t,x,\varphi(t,x)\big)\,\nabla\varphi(t,x)\Big) & \\ \qquad = q_4\left[\varphi(t,x) - \varphi^3(t,x)\right] + p_4 u(t,x) + q_5 g_2(t,x) & \text{in } Q \\ q_3\dfrac{\partial}{\partial \mathbf{n}}\varphi(t,x) = 0 & \text{in } \Sigma \\ \varphi(0,x) = \varphi_0(x) & \text{on } \Omega. \end{cases} \tag{6}$$

Within the framework of this section, we will approach the nonlinear parabolic system (5) and (6) in the spirit given by Hadamard's well-posedness conditions (see ([10], p. 46)). Consequently, our main result in studying problems (5) and (6) is the following

Theorem 1. *Problems* (5) and (6) *have a unique solution* $(u, \varphi) \in W_p^{2,1}(Q) \times W_\nu^{2,1}(Q)$, *where* $\nu = \min\{q, \mu\}$. *In addition, the pair function* (u, φ) *satisfies*

$$\begin{aligned} &\|u\|_{W_p^{2,1}(Q)} + \|\varphi\|_{W_\nu^{2,1}(Q)} \\ &\leq C\Big[1 + \|u_0\|_{W_p^{2-\frac{2}{p}}(\Omega)} + \|\varphi_0\|^{2-\frac{1}{q}}_{W_q^{2-\frac{2}{q}}(\Omega)} + \|g_{fr}\|_{W_p^{2-\frac{1}{p},1-\frac{1}{2p}}(\Sigma)} + \|g_1\|_{L^p(Q)} + \|g_2\|_{L^q(Q)}\Big] \end{aligned} \tag{7}$$

where the constant C *depends on* $|\Omega|$ *(the measure of* Ω*),* T, n, p, q*, and physical parameters.*

Moreover, given any number $N > 0$*, if* (u_1, φ_1)*,* (u_2, φ_2) *are solutions of* (5) *and* (6) *corresponding to the data* (g_1^1, g_2^1, g_{fr}^1)*,* $(g_1^2, g_2^2, g_{fr}^2) \in L^p(Q) \times L^q(Q) \times W_p^{2-\frac{1}{p},1-\frac{1}{2p}}(\Sigma)$*, respectively, for the same initial conditions, such that* $\|\varphi_1\|_{L^\nu(Q)}, \|\varphi_2\|_{L^\nu(Q)} \leq N$*, then the estimate below holds*

$$\begin{aligned} &\|u_1 - u_2\|_{W_p^{2,1}(Q)} + \|\varphi_1 - \varphi_2\|_{W_\nu^{2,1}(Q)} \\ &\leq C\left(\|g_1^1 - g_1^2\|_{L^p(Q)} + \|g_2^1 - g_2^2\|_{L^q(Q)} + \|g_{fr}^1 - g_{fr}^2\|_{W_p^{2-\frac{1}{p},1-\frac{1}{2p}}(\Sigma)}\right) \end{aligned} \tag{8}$$

where $C > 0$ *depends on* $|\Omega|, T, n, N, p, q$*, and the physical parameters.*

An Auxiliary Nonlinear Second-Order Boundary Value Problem

Before starting the proof of Theorem 1, we recall a result that concerns the existence and the uniqueness of the solution to an auxiliary nonlinear parabolic equation derived from (6). So, we consider the nonlinear second-order boundary value problem

$$\begin{cases} q_2 \dfrac{\partial}{\partial t}\varphi(t,x) - q_3 \mathrm{div}\Big(K(t,x,\varphi(t,x))\,\nabla\varphi(t,x)\Big) & \\ \qquad = q_4\left[\varphi(t,x) - \varphi^3(t,x)\right] + \bar{g}_2(t,x) & \text{in} \quad Q \\ q_3 \dfrac{\partial}{\partial \mathbf{n}}\varphi(t,x) = 0 & \text{in} \quad \Sigma \\ \varphi(0,x) = \varphi_0(x) & \text{on} \quad \Omega. \end{cases} \tag{9}$$

Definition 1. *Any solution* $\varphi(t,x)$ *of the problem* (9) *is called the* `classical solution` *if it is continuous in* $\bar{Q}$*, if it has continuous derivatives* $\varphi_t(t,x)$*,* $\varphi_x(t,x)$*,* $\varphi_{xx}(t,x)$ *in* Q*, if it satisfies the Equation* $(9)_1$ *at all points* $(t,x) \in Q$ *and satisfies the conditions* $(9)_2$ *and* $(9)_3$ *on the lateral surface* Σ *of the cylinder* Q *and for* $t = 0$*, respectively.*

The main results regarding the existence, uniqueness, and regularity of the solutions to problem (9) are as follows

Theorem 2. *Suppose that* $\varphi(t,x) \in C^{1,2}(Q)$ *is a classical solution of problem* (9) *and for positive numbers* M*,* M_0*,* m_1*,* M_1*,* M_2*,* M_3*,* M_4*, and* M_5*, one has*

$\mathbf{I}_1$. $|\varphi(t,x)| < M$ *for any* $(t,x) \in Q$ *and for any* $z(t,x)$*, the map* $K(t,x,z)$ *is continuous, differentiable in* x*, its* x*-derivatives are measurably bounded, and satisfies relation* (6) *in* [2] *and*

$$0 < K_{min} \leq K\big(t,x,\varphi(t,x)\big) < K_{max}, \quad \textit{for} \ \ (t,x) \in Q, \tag{10}$$

$$\sum_{i=1}^{n}\left[|a_i(t,x,\varphi(t,x),z(t,x))| + \left|\frac{\partial}{\partial\varphi}a_i(t,x,\varphi(t,x),z(t,x))\right|\right](1+|z|)$$
$$+\sum_{i,j=1}^{n}\left|\frac{\partial}{\partial x_j}a_i(t,x,\varphi(t,x),z(t,x))\right|+|\varphi(t,x)|\leq M_0(1+|z|)^2. \tag{11}$$

$\mathbf{I}_2$. *For any sufficiently small $\varepsilon > 0$, the functions $\varphi(t,x)$ and $K(t,x,\varphi(t,x))$ satisfy the relations*

$$\|\varphi\|_{L^s(Q)} \leq M_2, \qquad \|K(t,x,\varphi(t,x))U_{x_i}\|_{L^r(Q)} < M_3, \;\; i = 1,\ldots,n,$$

where

$$r = \begin{cases} \max\{p,4\} & p \neq 4 \\ 4+\varepsilon & p = 4, \end{cases} \qquad s = \begin{cases} \max\{p,2\} & p \neq 2 \\ 2+\varepsilon & p = 2. \end{cases}$$

Then, $\forall\ \bar{g}_2 \in L^p(Q)$, $\varphi_0 \in W_\infty^{2-\frac{2}{p}}(\Omega)$, with $p \neq \frac{3}{2}$, there exists a unique solution $\varphi \in W_p^{1,2}(Q)$ to (9) and satisfies

$$\|\varphi\|_{W_p^{1,2}(Q)} \leq C\left\{1 + \|\varphi_0\|_{W_\infty^{2-\frac{2}{p}}(\Omega)} + \|\varphi_0\|_{L^{3p-2}(\Omega)}^{\frac{3p-2}{p}} + \|\bar{g}_2\|_{L^{3p-2}(Q)}^{\frac{3p-2}{p}}\right\}, \tag{12}$$

where $C > 0$ does not depend on φ and $\bar{g}_2$.

If φ^1, φ^2 are solutions to (9) corresponding to $\varphi_0^1, \varphi_0^2 \in W_\infty^{2-\frac{2}{p}}(\Omega)$, $\bar{g}_2^1$ and $\bar{g}_2^2$, respectively, such that

$$\|\varphi^1\|_{W_p^{1,2}(Q)}, \quad \|\varphi^2\|_{W_p^{1,2}(Q)} \leq M_4, \tag{13}$$

then, the following holds

$$\max_{(t,x)\in Q}|\varphi^1 - \varphi^2| \leq C_1 e^{CT} \max\left\{\max_{(t,x)\in\Omega}|\varphi_0^1 - \varphi_0^2|, \max_{(t,x)\in Q}|\bar{g}_2^1 - \bar{g}_2^2|\right\}, \tag{14}$$

where $C_1 > 0$ and $C > 0$ do not depend on $\left\{\varphi^1, \bar{g}_2^1, \varphi_0^1,\right\}$ and $\left\{\varphi^2, \bar{g}_2^2, \varphi_0^2\right\}$. In particular, the uniqueness of the solution to (9) holds.

As far as the techniques used in the paper are concerned, it should be noted that we derive the a priori estimates in $L^p(Q)$. Moreover, the basic tools in our approach are:

- The Leray–Schauder degree theory (see ([1], p. 221) and reference therein);
- The L^p-theory of the linear and quasi-linear parabolic equations (see [1] and the reference therein);
- Green's first identity

$$-\int_\Omega y \,\mathrm{div} z\, dx = \int_\Omega \nabla y \cdot z\, dx - \int_{\partial\Omega} y \frac{\partial}{\partial\mathbf{n}} z\, d\gamma,$$
$$-\int_\Omega y \Delta z\, dx = \int_\Omega \nabla y \cdot \nabla z\, dx - \int_{\partial\Omega} y \frac{\partial}{\partial\mathbf{n}} z\, d\gamma, \tag{15}$$

for any scalar-valued function y and z, a continuously differentiable vector field in n-dimensional space;

- The Lions and Peetre embedding Theorem ([1], p. 14) to ensure the existence of a continuous embedding $W_p^{1,2}(Q) \subset L^\mu(Q)$, $p \geq 2$, where the number μ is defined as follows

$$\mu = \begin{cases} \text{any positive number } \geq 3p & \text{if } \dfrac{1}{p} - \dfrac{2}{n+2} \leq 0, \\ \dfrac{p\,(n+2)}{n+2-2p} & \text{if } \dfrac{1}{p} - \dfrac{2}{n+2} > 0. \end{cases} \tag{16}$$

For a given positive integer k and $1 \leq p \leq \infty$, we denote by $W_p^{k,2k}(Q)$ the Sobolev space on Q:

$$W_p^{k,2k}(Q) = \left\{ y \in L^p(Q) : \frac{\partial^i}{\partial t^i} \frac{\partial^j}{\partial x^j}\, y \in L^p(Q), \text{ for } 2i + j \leq 2k \right\},$$

i.e., the spaces of functions whose t-derivatives and x-derivatives are up to the orders of k and $2k$, respectively, belonging to $L^p(Q)$. Also, we will use the Sobolev spaces $W_p^i(\Omega)$, $W_p^{\frac{i}{2},i}(\Sigma)$ with a non-integral i for the initial and boundary conditions, respectively (see ([1], p. 14) and references therein).

Also, we shall use the set $C^{1,2}(\bar{D})$ ($C^{1,2}(D)$) of all continuous functions in $\bar{D}$ (in D) having continuous derivatives u_t, u_x, u_{xx} in $\bar{D}$ (in D) ($D = Q$ or $D = \Sigma$), as well as the Sobolev spaces $W_p^\ell(\Omega)$, $W_p^{\ell,\ell/2}(\Sigma)$ with non-integral ℓ for the initial and boundary conditions, respectively (see [2] and references therein).

The results in Theorem 2 are established in [2], which corresponds to a more general boundary condition. Here, we omit details of the proof.

Proof. Proof of the Theorem 1

We introduce the homotopy $J : L^p(Q) \times [0,1] \to L^p(Q)$ as follows

$$J(v, \lambda) = u, \quad \forall (v, \lambda) \in L^p(Q) \times [0,1], \tag{17}$$

where u is the unique solution of the linear problem

$$\begin{cases} p_1 \dfrac{\partial}{\partial t} u(t,x) - p_2 \Delta u(t,x) = \lambda \Big[-q_1 \dfrac{\partial}{\partial t} \varphi(t,x) + p_3 g_1(t,x) \Big] & \text{in } \quad Q \\ p_2 \dfrac{\partial}{\partial \mathbf{n}} u(t,x) + p_5 u(t,x) = \lambda g_{fr}(t,x) & \text{in } \quad \Sigma \\ u(0,x) = \lambda u_0(x) & \text{on } \quad \Omega, \end{cases} \tag{18}$$

with φ representing the unique solution of the nonlinear parabolic boundary value problem

$$\begin{cases} q_2 \dfrac{\partial}{\partial t} \varphi(t,x) - q_3 \mathrm{div}\Big(K\big(t,x,\varphi(t,x)\big)\, \nabla \varphi(t,x) \Big) & \\ \qquad\qquad = q_4 \left[\varphi(t,x) - \varphi^3(t,x) \right] + p_4 v(t,x) + q_5 g_2(t,x) & \text{in } \quad Q \\ q_3 \dfrac{\partial}{\partial \mathbf{n}} \varphi(t,x) = 0 & \text{in } \quad \Sigma \\ \varphi(0,x) = \varphi_0(x) & \text{on } \quad \Omega, \end{cases} \tag{19}$$

Since $p \leq q$ (see (2)), then $\bar{g}_2 = p_4 v(t,x) + q_5 g_2(t,x) \in L^p(Q)$. Using Theorem 2, we see that there exists a unique solution $\varphi \in W_p^{2,1}(Q)$ of (19) and thus $-q_1 \dfrac{\partial}{\partial t} \varphi(t,x) + p_3 g_1(t,x) \in L^p(Q)$. The L_p-theory guarantees that the linear parabolic Equation (18) has a unique solution $u \in W_p^{2,1}(Q)$. Hence, the mapping H introduced in (17) is well defined.

Next, following the same reasoning as in ([10], p. 53) we obtain (7) and (8).

The uniqueness of the solution $\{u, \varphi\}$ follows from (8) by taking $g_1^1 = g_1^2$, $g_2^1 = g_2^2$, $g_{fr}^1 = g_{fr}^2$ and so the proof of Theorem 1 is finished. $\square$

3. Approximating Scheme of Fractional Steps Type: The Phase-Field Transition System

The purpose of this section is to use the *fractional steps method* in order to approximate the unique solution of the nonlinear second-order parabolic systems (5) and (6), extending the result already studied in [2]. Namely, for every $\varepsilon > 0$, let

$$Q_i^\varepsilon = [i\varepsilon, (i+1)\varepsilon] \times \Omega, \quad \Sigma_i^\varepsilon = [i\varepsilon, (i+1)\varepsilon] \times \partial\Omega,$$

for $i = 0, 1, \cdots, M_\varepsilon - 1$, with $M_\varepsilon = \left[\frac{T}{\varepsilon}\right]$. Suitably, we associate the following numerical scheme with problems (5) and (6):

$$\begin{cases} p_1 \dfrac{\partial}{\partial t} u^\varepsilon(t,x) + q_1 \dfrac{\partial}{\partial t} \varphi^\varepsilon(t,x) = p_2 \Delta u^\varepsilon(t,x) + p_3 g_1(t,x) & \text{in} \quad Q_i^\varepsilon \\ p_2 \dfrac{\partial}{\partial \mathbf{n}} u^\varepsilon(t,x) + p_5 u^\varepsilon(t,x) = g_{fr}(t,x) & \text{on} \quad \Sigma_i^\varepsilon \\ u_+^\varepsilon(i\varepsilon, x) = u_-^\varepsilon(i\varepsilon, x), \quad u^\varepsilon(0,x) = u_0(x) & \text{on} \quad \Omega, \end{cases} \tag{20}$$

$$\begin{cases} q_2 \dfrac{\partial}{\partial t} \varphi^\varepsilon(t,x) - q_3 \mathrm{div}\Big(K\big(t,x,\varphi^\varepsilon(t,x)\big)\ \nabla \varphi^\varepsilon(t,x)\Big) & \\ \qquad\qquad = q_4 \varphi^\varepsilon(t,x) + p_4 u^\varepsilon(t,x) + q_5 g_2(t,x) & \text{in} \quad Q_i^\varepsilon \\ q_3 \dfrac{\partial}{\partial \mathbf{n}} \varphi^\varepsilon(t,x) = 0 & \text{in} \quad \Sigma_i^\varepsilon \\ \varphi^\varepsilon(i\varepsilon, x) = z(\varepsilon, \varphi_-^\varepsilon(i\varepsilon, x)) & \text{on} \quad \Omega, \end{cases} \tag{21}$$

where $z(\varepsilon, \varphi_-^\varepsilon(i\varepsilon, x))$ is the solution of the Cauchy problem:

$$\begin{cases} z'(s) + q_4 z^3(s) = 0 & s \in [0, \varepsilon] \\ z(0) = \varphi_-^\varepsilon(i\varepsilon, x) & \text{on} \ \ \Omega \\ \quad \varphi_-^\varepsilon(0,x) = \varphi_0(x) & \text{on} \ \ \Omega \end{cases} \tag{22}$$

for $i = 0, 1, \cdots, M_\varepsilon - 1$, where φ_-^ε stands for the left-hand limit of φ^ε.

For a detailed discussion regarding the importance of the above numerical scheme, we direct the reader to the works [1,10–12,14].

The main question of the whole work is that of the convergence of $\varepsilon \to 0$ of the sequence $(u^\varepsilon, \varphi^\varepsilon)$ of solutions to problems (20) and (21) to the solution (u, φ) of problems (5) and (6) (see [13,15,16]).

For later use, we set

$$W = L^2([0,T]; H^1(\Omega)) \cap W^{1,2}([0,T]; (H^1(\Omega))').$$

Definition 2. *By a weak solution to nonlinear systems (5) and (6), we refer to a pair of functions $u, \varphi \in W$, which satisfy (5) and (6) in the following sense:*

$$
\begin{aligned}
&\int\limits_Q \left(p_1 \frac{\partial}{\partial t} u + q_1 \frac{\partial}{\partial t} \varphi, \phi_1 \right) dt\, dx + p_2 \int\limits_Q \nabla u \nabla \phi_1 \, dt\, dx + p_5 \int\limits_\Sigma u \phi_1 \, dt\, d\gamma \\
&\quad = p_3 \int\limits_Q g_1 \phi_1 \, dtdx + \int\limits_\Sigma g_{fr} \phi_1 \, dt\, d\gamma,
\end{aligned} \tag{23}
$$

$$
\begin{aligned}
&q_1 \int\limits_Q \left(\frac{\partial}{\partial t} \varphi, \phi_2 \right) dt\, dx + q_3 \int\limits_Q K(t, x, \varphi) \nabla \varphi \cdot \nabla \phi_2 \, dt\, dx \\
&\quad = q_4 \int\limits_Q (\varphi - \varphi^3) \phi_2 \, dt\, dx + p_4 \int\limits_Q u \phi_1 \, dt\, dx + q_5 \int\limits_Q g_2 \phi_2 \, dtdx,
\end{aligned} \tag{24}
$$

$$
\forall \phi_1, \phi_2 \in L^2([0, T]; H^1(\Omega)),
$$

and $u(0, x) = u_0(x),\ \varphi(0, x) = \varphi_0(x)$ on Ω.

Definition 3. *By a weak solution to nonlinear systems (20) and (21), we refer to a pair of functions $u^\varepsilon, \varphi^\varepsilon \in W$ which satisfy (20) and (21) in the following sense:*

$$
\begin{aligned}
&\int\limits_Q \left(p_1 \frac{\partial}{\partial t} u^\varepsilon + q_1 \frac{\partial}{\partial t} \varphi^\varepsilon, \phi_1 \right) dt\, dx + p_2 \int\limits_Q \nabla u^\varepsilon \nabla \phi_1 \, dt\, dx + p_5 \int\limits_\Sigma u^\varepsilon \phi_1 \, dt\, d\gamma \\
&\quad = p_3 \int\limits_Q g_1 \phi_1 \, dtdx + \int\limits_\Sigma g_{fr} \phi_1 \, dt\, d\gamma,
\end{aligned} \tag{25}
$$

$$
\begin{aligned}
&q_1 \int\limits_Q \left(\frac{\partial}{\partial t} \varphi^\varepsilon, \phi_2 \right) dt\, dx + q_3 \int\limits_Q K(t, x, \varphi^\varepsilon) \nabla \varphi^\varepsilon \cdot \nabla \phi_2 \, dt\, dx \\
&\quad = q_4 \int\limits_Q \varphi^\varepsilon \phi_2 \, dt\, dx + p_4 \int\limits_Q u^\varepsilon \phi_1 \, dt\, dx + q_5 \int\limits_Q g_2 \phi_2 \, dtdx,
\end{aligned} \tag{26}
$$

$$
\forall \phi_1, \phi_2 \in L^2([0, T]; H^1(\Omega)),
$$

and $u^\varepsilon_-(0, x) = u_0(x),\ \varphi^\varepsilon_-(0, x) = \varphi_0(x)$ on Ω.

In (23)–(26), we denoted by the same symbol $\int\limits_Q$ the duality between

$$
L^2([0, T]; H^1(\Omega)) \text{ and } L^2([0, T]; (H^1(\Omega))').
$$

3.1. Convergence of the Fractional Steps Scheme (20) and (21)

The purpose of this subsection is to prove the convergence of the solution to the numerical schemes (20) and (21) associated with the phase-field transition systems (5) and (6). Therefore,

Theorem 3. *Assume that* $u_0, \varphi_0 \in W_p^{2-\frac{2}{p}}(\Omega)$, *with* $p_2 \frac{\partial}{\partial \nu} u_0 + p_5 u_0 = g_{fr}(0,x)$, $q_3 \frac{\partial}{\partial \nu} \varphi_0 = 0$ *on* $\partial\Omega$ *and* $g_{fr}(s,x) \in W_p^{1-\frac{1}{2p}, 2-\frac{1}{p}}(\Sigma)$. *Let* $(u^\varepsilon, \varphi^\varepsilon)$ *be the solution of the approximating scheme* (20) *and* (21). *As* $\varepsilon \to 0$, *one has*

$$(u^\varepsilon(s), \varphi^\varepsilon(s)) \to (u^*(s), \varphi^*(s)) \quad \text{strongly in } L^2(\Omega) \text{ for any } s \in (0,T], \tag{27}$$

where $u^*, \varphi^* \in W^{1,2}([0,T]; L^2(\Omega)) \cap L^2([0,T]; H^2(\Omega))$ *is the weak solution of the phase-field transition systems* (5) *and* (6).

The following lemmas (proven for the first time in the work [10]) which involve the Cauchy problem (22) are very useful in the proof of the main result of Theorem 3. Here, we reproduce them as well as sketch out the proof when pertinent.

Lemma 1. *Assume that* $\varphi_-^\varepsilon(i\varepsilon, x) \in L^\infty(\Omega)$, $i = 0, 1, ..., M_\varepsilon - 1$. *Then,* $\varphi^\varepsilon(i\varepsilon, x) \in L^\infty(\Omega)$ *and*

$$\|\varphi^\varepsilon(i\varepsilon, x)\|^2_{L^2(\Omega)} \leq \|\varphi_-^\varepsilon(i\varepsilon, x)\|^2_{L^2(\Omega)}. \tag{28}$$

Proof. We write $(22)_1$ in the form $\left(\dfrac{1}{z^2}\right)' = q_4$ and, following the same reasoning as in [1], we obtain

$$z^2(\varepsilon, \varphi_-^\varepsilon(i\varepsilon, x)) \leq \varphi_-^\varepsilon(i\varepsilon, x)^2, \quad a.e \;\; x \in \Omega. \tag{29}$$

Owing to $(21)_3$ and (29), it is easy to conclude the inequality complete in (28). □

Lemma 2. *For* $i = 0, 1, ..., M_\varepsilon - 1$, *the estimate below holds*

$$\|\nabla \varphi^\varepsilon(i\varepsilon, x)\|_{L^2(\Omega)} \leq \|\nabla \varphi_-^\varepsilon(i\varepsilon, x)\|_{L^2(\Omega)}. \tag{30}$$

Lemma 3. *The following estimate holds*

$$\|z(\varepsilon, x) - \varphi_-^\varepsilon(i\varepsilon, x)\|_{L^2(\Omega)} \leq \varepsilon L \tag{31}$$

where $L > 0$ *depends on* $|\Omega|$, $\|U_-^\varepsilon\|_{L^\infty(\Omega)}$ *and* p_2.

Proof of Theorem 3. Following the same steps as in [10], we obtain the solution to problem (21) as $\varphi^\varepsilon \in W_p^{1,2}(Q_i^\varepsilon) \cap L^\infty(Q_i^\varepsilon)$, $\forall i \in \{0, 1, ..., M_\varepsilon - 1\}$.

Then, we give a priori estimates in Q_i^ε, $\forall i \in \{0, 1, ..., M_\varepsilon - 1\}$. Multiplying $(20)_1$ by $\dfrac{p_4}{q_1} u^\varepsilon$, $(21)_1$ by φ_t^ε using the integration by parts, Green's formula, and the relations (25) and (26), we obtain

$$\begin{aligned} &\frac{p_4}{q_1}\frac{p_1}{2}\frac{d}{dt}\int_\Omega |u^\varepsilon|^2 dx + p_4 \int_\Omega u^\varepsilon \varphi_t^\varepsilon dx + \frac{p_4}{q_1} p_2 \int_\Omega |\nabla u^\varepsilon|^2 dx + \frac{p_4}{q_1} p_5 \int_{\partial\Omega} |u^\varepsilon|^2 d\gamma \\ &\qquad = \frac{p_4}{q_1} p_3 \int_\Omega g_1 u^\varepsilon \, dx + \frac{p_4}{q_1} \int_{\partial\Omega} g_{fr} u^\varepsilon \, d\gamma, \end{aligned} \tag{32}$$

$$\begin{aligned} &q_2 \int_\Omega |\varphi_t^\varepsilon|^2 dx + \frac{q_3}{2} \int_\Omega K(t, x, \varphi^\varepsilon) \frac{d}{dt} |\nabla \varphi^\varepsilon|^2 dx \\ &\qquad = \frac{q_4}{2}\frac{d}{dt}\int_\Omega |\varphi^\varepsilon|^2 dx + p_4 \int_\Omega u^\varepsilon \varphi_t^\varepsilon dx + q_5 \int_\Omega g_2 \, \varphi_t^\varepsilon \, dx. \end{aligned} \tag{33}$$

Using Hölder's inequality for the right terms $\frac{p_4}{q_1} p_3 \int_\Omega g_1 u^\varepsilon \, dx$, $\frac{p_4}{q_1} \int_{\partial\Omega} g_{fr} u^\varepsilon \, d\gamma$ and $q_5 \int_\Omega g_2 \, \varphi_t^\varepsilon \, dx$, we have

$$\frac{p_4}{q_1} p_3 \int_\Omega g_1 u^\varepsilon \, dx \le \frac{1}{2} \int_\Omega |u^\varepsilon|^2 \, dx + \frac{p_4}{q_1} \frac{p_3}{2} \int_\Omega |g_1|^2 \, dx,$$

$$\frac{p_4}{q_1} \int_{\partial\Omega} g_{fr} u^\varepsilon \, d\gamma \le \frac{p_4}{q_1} p_5 \int_{\partial\Omega} |u^\varepsilon|^2 d\gamma + \frac{p_4}{q_1} \frac{1}{p_5} \int_{\partial\Omega} |g_{fr}|^2(t,x) d\gamma,$$

$$q_5 \int_\Omega g_2 \, \varphi_t^\varepsilon \, dx \le \frac{q_2}{2} \int_\Omega |\varphi_t^\varepsilon|^2 \, dx + \frac{q_5}{2q_2} \int_\Omega |g_2|^2 \, dx.$$

Adding (32) and (33) and making use of the last inequality, we obtain:

$$\begin{aligned} &\frac{p_4}{q_1} \frac{p_1}{2} \frac{d}{dt} \int_\Omega |u^\varepsilon|^2 dx + \frac{p_4}{q_1} p_2 \int_\Omega |\nabla u^\varepsilon|^2 dx + \frac{q_2}{2} \int_\Omega |\varphi_t^\varepsilon|^2 \, dx + \frac{q_3}{2} K_{min} \frac{d}{dt} \int_\Omega |\nabla \varphi^\varepsilon|^2 dx \\ &\le \frac{q_4}{2} \frac{d}{dt} \int_\Omega |\varphi^\varepsilon|^2 dx + \frac{1}{2} \int_\Omega |u^\varepsilon|^2 \, dx \\ &+ \frac{p_4}{q_1} \frac{p_3}{2} \int_\Omega |g_1|^2 \, dx + \frac{q_5}{2q_1} \int_\Omega |g_2|^2 \, dx + \frac{p_4}{q_1} \frac{1}{p_5} \int_{\partial\Omega} |g_{fr}|^2(t,x) d\gamma, \end{aligned} \tag{34}$$

where the inequality (10) has also been used.

Now, multiplying $(21)_1$ by $\frac{2q_4}{q_2} \varphi^\varepsilon$ as shown above, we obtain

$$\begin{aligned} &q_4 \frac{d}{dt} \int_\Omega |\varphi^\varepsilon|^2 dx + \frac{2q_4}{q_2} q_3 \int_\Omega K(t,x,\varphi^\varepsilon) |\nabla \varphi^\varepsilon|^2 dx \\ &= \frac{2q_4}{q_2} q_4 \int_\Omega |\varphi^\varepsilon|^2 dx + \frac{2q_4}{q_2} p_4 \int_\Omega u^\varepsilon \varphi^\varepsilon dx + \frac{2q_4}{q_2} q_5 \int_\Omega g_2 \, \varphi^\varepsilon \, dx. \end{aligned} \tag{35}$$

Again, using Hölder's inequality for the right terms $\int_\Omega u^\varepsilon \varphi^\varepsilon dx$ and $\int_\Omega g_2 \, \varphi^\varepsilon \, dx$, we have

$$\frac{2q_4}{q_2} p_4 \int_\Omega u^\varepsilon \varphi^\varepsilon dx \le \frac{2q_4}{2q_2} p_4 \int_\Omega |u^\varepsilon|^2 \, dx + \frac{2q_4}{2q_2} p_4 \int_\Omega |\varphi^\varepsilon|^2 \, dx,$$

$$\frac{2q_4}{q_2} q_5 \int_\Omega g_2 \, \varphi^\varepsilon \, dx \le \frac{2q_4}{2q_2} q_5 \int_\Omega |\varphi^\varepsilon|^2 \, dx + \frac{2q_4}{2q_2} q_5 \int_\Omega |g_2|^2 \, dx,$$

and then, from (35), we obtain

$$\begin{aligned} &q_4 \frac{d}{dt} \int_\Omega |\varphi^\varepsilon|^2 dx + \frac{2q_4}{q_2} q_3 K_{min} \int_\Omega |\nabla \varphi^\varepsilon|^2 dx \\ &\le C(q_2, q_3, q_4, p_4, q_5) \left[\int_\Omega |u^\varepsilon|^2 dx + \int_\Omega |\varphi^\varepsilon|^2 dx + \int_\Omega |g_2|^2 dx \right], \end{aligned} \tag{36}$$

where the inequality (10) has also been used.

Adding (34) and (36), we obtain

$$\frac{\partial}{\partial t}\left[\frac{p_4}{q_1}\frac{p_1}{2}\int_\Omega |u^\varepsilon|^2dx + \frac{q_4}{2}\int_\Omega |\varphi^\varepsilon|^2dx + \frac{q_3}{2}K_{min}\int_\Omega |\nabla\varphi^\varepsilon|^2dx\right]$$

$$+\frac{q_1}{2}\int_\Omega |\varphi_t^\varepsilon|^2dx + \frac{p_4}{q_1}p_2\int_\Omega |\nabla u^\varepsilon|^2dx + \frac{2q_4}{q_2}q_3K_{min}\int_\Omega |\nabla\varphi^\varepsilon|^2dx$$

$$\leq C(p_1,p_2,p_3,p_4,p_5,q_1,q_2,q_3,q_4,q_5)\left[\int_\Omega |u^\varepsilon|^2dx + \int_\Omega |\varphi^\varepsilon|^2dx\right.$$

$$\left.+\int_\Omega |g_1|^2\,dx + \int_\Omega |g_2|^2dx + \int_{\partial\Omega} |g_{fr}|^2(t,x)d\gamma\right].$$

Integrating the preceding on Q_i^ε, $i = 0,1,2,...,M_\varepsilon - 1$ (i.e., on $[i\varepsilon,(i+1)\varepsilon]$, $i = 0,1,2,...,M_\varepsilon - 1$) and summing the inequalities obtained, we derive (see ([10], p. 102), for example)

$$\frac{p_4}{q_1}\frac{p_1}{2}\|u_-^\varepsilon(T,x)\|^2_{L^2(\Omega)} + \frac{q_4}{2}\|\varphi_-^\varepsilon(T,x)\|^2_{L^2(\Omega)} + \frac{q_3}{2}K_{min}\|\nabla\varphi_-^\varepsilon(T,x)\|^2_{L^2(\Omega)}$$

$$+\int_0^T\left[\frac{q_1}{2}\|\varphi_t^\varepsilon\|^2_{L^2(\Omega)} + \frac{p_4}{q_1}p_2\|\nabla u^\varepsilon\|^2_{L^2(\Omega)} + \frac{2q_4}{q_2}q_3K_{min}\|\nabla\varphi^\varepsilon\|^2_{L^2(\Omega)}\right]dt$$

$$\leq \frac{p_4}{q_1}\frac{p_1}{2}\|u_0\|^2_{L^2(\Omega)} + \frac{q_4}{2}\|\varphi_0\|^2_{L^2(\Omega)} + \frac{p_2}{2}\|\nabla U_0\|^2_{L^2(\Omega)} + \frac{q_3}{2}K_{min}\|\nabla\varphi_0\|^2_{L^2(\Omega)}$$

$$+C(p_1,p_2,p_3,p_4,p_5,q_1,q_2,q_3,q_4,q_5)\left\{\int_0^T\left[\|u^\varepsilon\|^2_{L^2(\Omega)} + \|\varphi^\varepsilon\|^2_{L^2(\Omega)}\right]dt\right.$$

$$\left.+\int_\Omega |g_1|^2\,dx + \int_\Omega |g_2|^2dx + \int_{\partial\Omega} |g_{fr}|^2(t,x)d\gamma\right\}.$$

where the inequalities (28) and (30) have also been used.

Applying Gronwall inequality to the above inequality, we finally deduce

$$\int_0^T\left\{\|\varphi_t^\varepsilon\|^2_{L^2(\Omega)} + \|\nabla u^\varepsilon\|^2_{L^2(\Omega)} + \|\nabla\varphi^\varepsilon\|^2_{L^2(\Omega)}\right\}dt \leq C, \tag{37}$$

where $C > 0$ is independent of ε and M_ε.

Owing to $(20)_3$, $(21)_3$ and (31), we obtain

$$\sum_{i=0}^{M_\varepsilon-1}\|u^\varepsilon(i\varepsilon,x) - u_-^\varepsilon(i\varepsilon,x)\|_{L^2(\Omega)} \leq TL = C_1, \tag{38}$$

$$\sum_{i=0}^{M_\varepsilon-1}\|\varphi^\varepsilon(i\varepsilon,x)-\varphi^\varepsilon_-(i\varepsilon,x)\|_{L^2(\Gamma)}\leq C_2, \tag{39}$$

where $C_1>0$, $C_2>0$ are independent of M_ε and ε. Summing (38) and (39), we obtain

$$\overset{T}{\underset{0}{V1}}\,u^\varepsilon+\overset{T}{\underset{0}{V2}}\,\varphi^\varepsilon+\int_0^T\Big[\|\varphi^\varepsilon_t\|^2_{L^2(\Omega)}+\|\nabla u^\varepsilon\|^2_{L^2(\Omega)}+\|\nabla\varphi^\varepsilon\|^2_{L^2(\Omega}\Big]ds\leq C, \tag{40}$$

where the positive constant C is independent on M_ε and ε, while $\overset{T}{\underset{0}{V1}}\,u^\varepsilon$, $\overset{T}{\underset{0}{V2}}\,\varphi^\varepsilon$, stand for the variation of $u^\varepsilon:[0,T]\to L^2(\Omega)$ and $\varphi^\varepsilon:[0,T]\to L^2(\Omega)$, respectively.

Now, multiplying $(20)_1$ by u^ε_t, integrating over $[i\varepsilon,(i+1)\varepsilon]$, $i=0,1,\cdots,M_\varepsilon-1$, and involving Cauchy–Schwartz's inequalities, Hölder's inequality, Cauchy's inequality, Gronwall–Bellman's inequality, as well as Green's formula, we finally obtain the estimate:

$$\frac{p_1}{2}\int_0^t\int_\Omega(u^\varepsilon_t)^2dxds+\frac{p_2}{2}\int_\Omega|\nabla u^\varepsilon|^2dx+\frac{p_2p_5}{4}\int_{\partial\Omega}(u^\varepsilon)^2d\gamma\leq C, \tag{41}$$

for all $\varepsilon>0$, where the constant $C>0$ does not depend on M_ε and ε.

Combining (40) with (41), we find that

$$\overset{T}{\underset{0}{V1}}\,u^\varepsilon+\overset{T}{\underset{0}{V2}}\,\varphi^\varepsilon+\int_0^T\Big[\|u^\varepsilon_t\|^2_{L^2(\Omega)}+\|\varphi^\varepsilon_t\|^2_{L^2(\Omega)}+\|\nabla u^\varepsilon\|^2_{L^2(\Omega)}+\|\nabla\varphi^\varepsilon\|^2_{L^2(\Omega}\Big]ds\leq C. \tag{42}$$

Since the injection of $L^2(\Omega)$ into $H^{-1}(\Omega)$ is compact and $\{u^\varepsilon_s(s)\}$, $\{\varphi^\varepsilon_s(s)\}$ are bounded in $L^2(\Omega)$ $\forall s\in[0,T]$, we conclude that there exists a bounded variation function: $u^*(s)\in BV([0,T];H^{-1}(\Omega))$, $\varphi^*(s)\in BV([0,T];H^{-1}(\Omega))$, respectively, and the subsequences $u^\varepsilon(s)$, $\varphi^\varepsilon(s)$ (see [10]) such that

$$u^\varepsilon(s)\to u^*(s)\quad\text{strongly in}\quad H^{-1}(\Omega)\quad\forall s\in[0,T], \tag{43}$$

$$\varphi^\varepsilon(s)\to\varphi^*(s)\quad\text{strongly in}\quad H^{-1}(\Omega)\quad\forall s\in[0,T]. \tag{44}$$

Furthermore, from (40), we deduce that

$$\begin{cases}u^\varepsilon\to u^* & weakly\ \ in\ \ L^2(0,T;H^1(\Omega)),\\ \varphi^\varepsilon\to\varphi^* & weakly\ \ in\ \ L^2(0,T;H^1(\Omega)).\end{cases} \tag{45}$$

By the well-known embeddings $H^1(\Omega)\subset L^2(\Omega)\subset H^{-1}(\Omega)$, standard interpolation inequalities (see ([10], p. 17)) yield that $\forall\ell>0$, $\exists C(\ell)>0$ such that

$$\begin{cases}\|u^\varepsilon(s)-u^*(s)\|_{L^2(\Omega)}\leq\ell\|u^\varepsilon(s)-u^*(s)\|_{H^1(\Omega)}+C(\ell)\|u^\varepsilon(s)-u^*(s)\|_{H^{-1}(\Omega)},\\ \|\varphi^\varepsilon(s)-\varphi^*(s)\|_{L^2(\Omega)}\leq\ell\|\varphi^\varepsilon(s)-\varphi^*(s)\|_{H^1(\Omega)}+C(\ell)\|\varphi^\varepsilon(s)-\varphi^*(s)\|_{H^{-1}(\Omega)},\end{cases} \tag{46}$$

$\forall\varepsilon>0$ and $\forall s\in[0,T]$, where $C(\ell)\to0$ as $\ell\to0$.

Finally, relations (43)–(46) permit us to conclude that the assertion performed in (27) holds true, ending the proof of Theorem 3. □

Corollary 1. *Assume that* $u_0, \varphi_0 \in W_p^{2-\frac{2}{p}}(\Omega)$ *with* $p_2 \frac{\partial}{\partial \nu} u_0(x) + p_5 u_0(x) = g_{fr}(0, x)$, $q_3 \frac{\partial}{\partial \nu} \varphi_0(x) = 0$ *on* $\partial\Omega$ *and* $g_{fr} \in W_p^{1-\frac{1}{2p}, 2-\frac{1}{p}}(\Sigma)$. *Then,* $u^\star, \varphi^* \in W$ *is a weak solution of the nonlinear second-order parabolic system* (1) + (3) + (4).

The general framework of the numerical algorithm to compute the approximate solution of the problem (1) + (3) + (4) via the *fractional steps scheme* may be demonstrated as follows:

Begin **alg-frac_sec-ord-varphi_PHT**
 $i := 0 \;\; \to u_0$ from $(20)_3$ and φ_0 from $(22)_3$;
 For $i := 0$ to $M_\varepsilon - 1$ do
  Compute $z(\varepsilon, \cdot)$ from (22);
  $\varphi^\varepsilon(i\varepsilon, \cdot) := z(\varepsilon, \cdot)$;
  Compute $(u^\varepsilon((i+1)\varepsilon, \cdot), \varphi^\varepsilon((i+1)\varepsilon, \cdot))$ solving the linear system
   $(20)_{1-2}$ + $(21)_{1-2}$;
 End-for;
End.

3.2. *Example of Numerical Implementation to* **alg-frac_sec-ord-varphi_PHT**

Here, we consider a particular case of parameters $p_1, p_2, p_3, p_4, q_1, q_2, q_3, q_4$ and q_5 in (1) + (3), namely:

$p_1 = \rho V$, ρ—the density, V—the casting speed;
$p_2 = k$, k—the thermal conductivity;
$p_3 = 0$;
$p_4 = \dfrac{m[S]_E}{2\sigma} T_E$, (see [11]);
$p_5 = h$, h—the heat transfer coefficient;
$q_1 = \dfrac{\ell}{2}$, ℓ—the latent heat;
$q_2 = \alpha\xi$, α—the relaxation time, ξ—the measure of the interface thickness;
$q_3 = 1$, $K(t, x, \varphi(t, x)) = \xi$;
$q_4 = \dfrac{1}{2\xi}$;
$q_5 = 0$;
$g_{fr}(t, x) = w_1(t, x) \;\; (t, x) \in Q$.

Correspondingly, the following nonlinear parabolic system

$$\begin{cases} \rho V \dfrac{\partial}{\partial t} u + \dfrac{\ell}{2} \dfrac{\partial}{\partial t} \varphi = k \Delta u \\[2ex] \alpha\xi \dfrac{\partial}{\partial t} \varphi = \xi \Delta \varphi + \dfrac{1}{2\xi}(\varphi - \varphi^3) + s_\xi u \end{cases} \quad \text{in } Q, \tag{47}$$

with the non-homogeneous Cauchy–Neumann boundary conditions

$$\begin{cases} k \dfrac{\partial}{\partial \nu} u + hu = w_1(t, x) \\[2ex] \xi \dfrac{\partial}{\partial \nu} \varphi = 0 \end{cases} \quad \text{on } \Sigma = (0, T] \times \partial\Omega, \tag{48}$$

and with the initial conditions (4), is obtained. (47) + (48) + (4) represents the mathematical model called the **phase field transition system**, introduced by Caginalp (see [5]) to model the transition between the solid and liquid phase in the melting/solidification process to a matter occupying a region Ω (see [1,4,6–11,17–22]). A finite element method (**fem**) (see [23]) is used to construct the numerical model (as can be seen in ([11], relation (4.5))) and an industrial implementation of (1) + (3) + (4), in this particular case, is presented in [11].

4. Conclusions

The main problem studied in this paper is a nonlinear second-order parabolic system (1), (3), and (4), with respect to the unknown functions $u(t,x)$ and $\varphi(t,x)$, emphasizing that the principal part is in *divergence* form for the unknown function $\varphi(t,x)$, $(t,x) \in Q$. Provided that the initial and boundary data meet appropriate regularity as well as compatibility conditions, the well posedness of a classical solution to the nonlinear problem is proven in this new formulation (Theorem 1). Precisely, the Leray–Schauder principle as well as the L^p theory of the linear and quasi-linear parabolic equations are involved to prove the qualitative properties of the solution $(u(t,x), \varphi(t,x))$. Moreover, the a priori estimates are made in $L^p(Q)$ which allow one to derive the regularity properties of higher order, namely $\Big(u(t,x), \varphi(t,x)\Big) \in W^{1,2}_p(Q) \times W^{1,2}_\nu(Q)$, $\nu = \min\{q, \mu\}$ (see (2) and (16)). Let us remark that, due to the presence of the terms $K(t,x,\varphi(t,x))$, the nonlinear operator J (see (17)) does not represent the gradient of the energy functional. Therefore, the new proposed second-order nonlinear system (1) + (3) + (4) cannot be obtained from the minimization of any energy cost functional, i.e., (1) is not a variational PDE model.

Next, an iterative scheme of the fractional steps type is introduced to approximate problems (5) and (6). The convergence result is established for the proposed numerical scheme, and a conceptual numerical algorithm, **alg-frac_sec-ord-varphi_PHT**, is formulated in the end. An example of the numerical implementation of the principal step in the conceptual algorithm **alg-frac_sec-ord-varphi_PHT**, that is:

Compute $(u^\varepsilon((i+1)\varepsilon,\cdot), \varphi^\varepsilon((i+1)\varepsilon,\cdot))$ *solving the linear system* $(20)_{1-2}$ + $(21)_{1-2}$,

is reported.

The qualitative results obtained here can later be involved in the quantitative approaches of the mathematical model (1) + (3) + (4) as well as in the study of distributed and/or boundary nonlinear optimal control problems governed by such a nonlinear problem. The numerical implementation of the conceptual algorithm, **alg-frac_sec-ord-varphi_PHT**, as well as various simulations regarding the physical phenomena described by then nonlinear parabolic problem (1), especially that corresponding to the different choice of mobility functions $K(t,x,\varphi(t,x))$ (see [3]), representing a matter for further investigation.

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