Preface

Last years have shown a great interest in studying applied mathematics problems. One of the most important classes of such problems is the class of systems with phase change (systems with free boundary) encountered in numerous problems of physics, such as: melting ice, crystal formation, diffusion of oxygen in an absorbent tissue, solidification in continuous casting, etc.

From mathematical point of view, a *free boundary problem* can be considered as a nonlinear parabolic equation with limit values, for which is unknown the solution and its field.

In mathematics literature, for the phenomenon of solidification are known more mathematical models designed to describe the free boundary. Remember in this connection the Stefan problem as well as the phase-field transition system (Caginalp's model). Among the papers and monographs devoted to the study of free boundary problems of Stefan type, we recall those signed by V. Barbu [1], V. Barbu & N. Barron [2], J.L. Lions [3], C. Saguez [4], V. Arnăutu & P. Neittaanmäki [5] and D. Tiba [6].

The phase-field transition system, known also as a *phase-field system*, was introduced in literature by G. Caginalp [7]. This model has been established as an extension (a refinement) of the classical two phase Stefan problem to capture the effects of *surface tension*, *supercooling*, *superheating*, etc. Phase-field model (often called as *phase-field transition system*) in the form in which it was introduced by Caginalp [7], consists in the following two nonlinear differential equations of parabolic type ($Q = [0, T] \times \Omega$):

$$u_t + \frac{\ell}{2}\varphi_t = k\Delta u + f \qquad \text{in } \ Q, \tag{1}$$

$$\tau\varphi_t = \xi^2\Delta\varphi + \frac{1}{2a}(\varphi - \varphi^3) + 2u + g \qquad \text{in } \ Q, \tag{2}$$

subject to the boundary conditions

$$u = u_\partial(x), \qquad \varphi = \varphi_\partial(x) \qquad\qquad x \in \partial\Omega, \tag{3}$$

and initial conditions

$$u(0,x) = u_0(x), \qquad \varphi(0,x) = \varphi_0(x) \qquad x \in \Omega, \tag{4}$$

where u, φ are the unknown functions, $f = g = 0$, and $\Omega, T, \ell, k, \tau, \xi, a$, are described in detail in Chapter 2.

On the one hand, the content of this book is dedicated to the approximation (from theoretical and numerical point of view) of equations (1)-(2) in the presence of different types of boundary conditions and, on the other hand, analysis of some boundary optimal control problems, governed by this system.

The present work is conceived on the basis of the results and methods used by the author in notes [8]-[37] and it consists in a preface, five chapters, two annexes and bibliography.

Several types of boundary conditions were considered in the context of this work, namely ($\Sigma = [0,T] \times \partial\Omega$):

$$\frac{\partial}{\partial\nu}u + hu = w(t,x), \qquad \frac{\partial}{\partial\nu}\varphi = 0 \quad \text{on} \quad \Sigma, \tag{3'}$$

$$\frac{\partial}{\partial\nu}u + hu = w(t)g(x), \qquad \varphi = 1 \quad \text{on} \quad \Sigma, \tag{3''}$$

$$\frac{\partial}{\partial\nu}u + hu = 0, \qquad \varphi = 0 \quad \text{on} \quad \Sigma, \tag{3'''}$$

$$\frac{\partial}{\partial\nu}u = 0, \qquad \frac{\partial}{\partial\nu}\varphi = 0 \quad \text{on} \quad \Sigma, \tag{3^{\rm iv}}$$

$$u = 0, \qquad \varphi = 0 \quad \text{on} \quad \Sigma. \tag{3^{\rm v}}$$

In the first sections of Chapter 1 we recall notations, definitions and the main spaces of functions, some results about approximation of the nonlinear equations in Banach spaces and basic notions from numerical analysis, etc, frequently used in the next chapters. In the last two sections of this chapter we present a more detailed descriptions about the phase-field system and about the continuous-casting process of steel - the main industrial technology involved in our numerical experiments.

In Chapter 2 we will deal, on one hand, with the study of the existence, uniqueness, regularity, and estimates of the solution of phase-field transition system and, on the other hand, we will analyze the convergence of some approximating schemes of fractional steps type associated with this nonlinear system. Section 2.1 studies is the existence, uniqueness and regularity of the solution of the phase-field transition system subject to the non-homogeneous Cauchy-Neumann boundary conditions (**Theorem 2.1**). Such kind of conditions allow to the phase-field system (Caginalp's model) to be considered as a model of heat transfer from the surface of product to the environment, when we assume that the heat is extracted by convection and conduction in the continuous casting process. The purpose of Section 2.2 is to treat the phase-field system with a general nonlinearity in φ. The existence, uniqueness, regularity and estimates of the solution it is proved (**Theorem 2.3**) for this relevant case. Basic tools in this approach are the Leray-Schauder degree theory, the L_p-theory of linear parabolic equations, properties of the Nemytskij operator, and a priori estimates in $L^p(Q)$. Section 2.3 reviews a fractional steps scheme corresponding to (1), (2), (3^{v}) and (4), with $f = g = 0$. The obtained result is included in **Proposition 2.1** and the idea of the proof is inspired from the work of V. Barbu & M. Iannelli [38]. The next Section is devoted to the extension of some results known for m-accretive operators (see, e.g., Barbu [39] and Brézis [40]) to ω-m-accretive operators (**Theorem 2.4**), with a fixed real number ω. As an application of the Theorem 2.4, it is shown how the nonlinear phase-field transition system (with homogeneous Neumann-Neumann boundary conditions - (3^{iv})) can be decoupled in two simples systems. In the last Sections of Chapter 2 we consider the phase-field transition system (1)-(2) and (4) with two different boundary conditions:

- homogeneous Cauchy-Dirichlet boundary conditions - ($3^{'''}$);
- non-homogeneous Cauchy-Neumann boundary conditions - ($3'$).

The main results are included in **Theorem 2.5** and **Theorem 2.6**, and assert that (in certain assumptions on data u_0, φ_0 and w) for $\varepsilon > 0$, the solution $(u^\varepsilon, \varphi^\varepsilon)$ of approximating scheme converge to the weak solution (u^*, φ^*) of problem (1), (2), (4) and ($3'''$) or ($3'$), respectively. It is also proved that the weak solution of approximating scheme is a strong solution; we are thus in front of a constructive way to demonstrate the existence solution in phase-field transition system. The methods used in demonstration of this convergence results are those of compactness (in particular Helly-Foias theorem). The weak stability of approximating scheme corresponding to boundary conditions ($3^{'''}$), is also proved (**Corollary 2.1**).

Some types of boundary optimal control problems, governed by the nonlinear phase-field transition system, are introduced and analyzed in

Chapter 3. The aim of the Section 3.1 is to prove (for later use) a priori estimates in $L^2([0,T];H^2(\Omega))$ for unknown u,φ in phase-field system, in the presence of following boundary conditions: $\frac{\partial}{\partial\nu}u+hu=w(t,x)$, $\frac{\partial}{\partial\nu}\varphi=0$ on Σ and, $\frac{\partial}{\partial\nu}u+hu=w(t)g(x)$, $\varphi=1$ on Σ, where $w:\Sigma\to I\!R$ (or $w:[0,T]\to I\!R$) represents *the boundary control* (the temperature of the surrounding at $\partial\Omega$). Both cases (w depending explicitly on t and x or only on t) allow the model of phase-field to be involved in realistic numerical simulations in the metallurgic industry, and not only.

In Section 3.2 we will prove the existence of an optimal control (**Proposition 3.3**) for the problem stated there. The proof of this result is based on estimates established in the previous Section. The distributed optimal control problem governed by phase-field system has been analyzed in works done by: Z. Chen & K.-H. Hoffmann [41], M. Heinkenschloss & E.W. Sachs [42], M. Heinkenschloss & F. Troltzsch [43], as well as K.-H. Hoffmann & L. Jiang [44]. Boundary optimal control problem governed by the classical Stefan problem in two phases was studied by V. Barbu [1], A. Friedman [45], C. Saguez [4], D. Tiba [6].

We associate to the optimal control problem introduced in 3.2 an approximating optimal control problem for which we prove, first, the existence of an optimal control. Besides the existence of an optimal control, the convergence of the optimal solution of approximating problem to the optimal solution of the original problem is proved in the Section 3.3. The result is included in (**Theorem 3.1**). For the approximating problem, necessary optimality conditions (**Theorem 3.2**) are established in the next Section. Such a problem was studied, for an optimal control problem governed by nonlinear and parabolic variational inequalities by V. Barbu in [46].

In Section 3.5 is defined another type of boundary optimal control problem (an inverse problem). Necessary optimality conditions (maximum principle) for such sort of problem are given by **Theorem 3.4**. A likewise problem was studied in V. Arnăutu [47] but governed by the Stefan problem.

An optimal control problem, with the distributed control acting on a subset $\omega\subset\Omega$ and with the state constraint in time variable (P_S), is analyzed in Section 3.6. The necessary optimality conditions for (P_S), **Theorem 3.5**, were obtained by passing to the limit for $\varepsilon\to 0$ in the approximating control process considered (the adequate penalty problem P_S^ε, $\varepsilon>0$).

The last Section of this Chapter is dedicated to a non-homogeneous boundary optimal control problem (P). The main result of this Section (**Theorem 3.6**) amounts to saying that problem (P) can be approximated for $\varepsilon \to 0$ by the sequence of problems (P^{ε}). The convergence of the approximating process leads to an idea of numerical approximation of the optimal control of problem (P), namely (see Chapter 4, algorithm `cpht-2D`, step **P2**), at every iteration *iter*, the computation of the approximate solution corresponding to the nonlinear phase-field transition system is substituted by computation of the approximate solution for an ordinary equation and a linear system. Hence a large amount of time is saved concerning computations.

Chapter 4 is oriented to the numerical analysis of the problems stated in Chapters 2 and 3.[1]

The first Section is dedicated to the approximation of solution to the phase-field system in 1D. The discrete state equations were constructed using a *First-order Implicit Backward Difference Formula* (**1-IMBDF**), (see and S.J. Ruuth [48]). Three numerical methods to compute the approximate solution (*Newton method*, the *fractional steps method* and *cubic spline method*) are developed and, corresponding, conceptual algorithms are presented (`algnewton1D`, `algfrac1D`, `algspline1D`). The use of the *fractional steps method* simplifies the numerical computation due to its decoupling feature (compares the algorithms `algnewton1D` and `algfrac1D`). Stability conditions (**Proposition 4.1**, **Proposition 4.2**) for fractional and cubic spline approximation are established too.

Section 4.2 deals with the approximation of solution to the phase-field system in 2D via fractional steps method. An implicit (backward) finite difference scheme in time and a **f**inite **e**lement **m**ethod (**fem**) in space are used to construct the discrete equations. An conceptual algorithm (`algfracfem2D`) have been introduced in order to compute the approximate solution.

In the next Section we will deal with the approximation of the boundary optimal control in $(\mathrm{P}^{\varepsilon}_{inv})$ stated by Theorem 3.4 in Section 3.5. The main novelty brought by the conceptual algorithm `InvPHT1D` is that the computation of the approximate solution corresponding to the nonlinear system (4.1) is replaced by the calculation of the approximate solution for an ordinary equation and a linear system (compare step **P1** in C. Moroşanu [14] with the steps **P1-P2** in the present algorithm). Numerical experiments join the abstract treatment.

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Two conceptual algorithms of gradient type (`scpth-2D`, `cpth-2D`) to compute the optimal control (see Theorem 3.5) and the suboptimal control (see Theorem 3.7) of problems (P_S) and (P^ε), introduced in Chapter 3, are presented at the end of this Chapter. Each algorithm is implemented and accompanied by numerical experiments.

Aspects of the implementation of conceptual algorithms developed in Chapter 4 and numerical results obtained through their use, are given in the last Chapter. Thus the reader may be convinced on the accuracy of programs written and can easily understand the importance of methods developed in this material. All programs were written in MATLAB language and are endowed with sufficient comments for facilitate tracking them.

We complete the work with two annexes. The existence and regularity for the solution of one linear system (*auxiliary linear system*), having a structure similar with those in the associated approximating schemes of nonlinear phase-field transition system, it is proved in ANNEXE A (**Theorem A.1**). Concerning the methods used in the proof, an essential difference with respect to Chapter 2 consists in that here we make a priori estimates in $L^2(Q)$ instead of $L^p(Q)$. The estimation technique used is also different from those used for the rest of the book. In ANNEXE B we have presented details about the implementation of the **fem** (**f**inite **e**lement **m**ethod).

Optimal control problems treated in this work reflect the continuous casting process of steel. To emphasize more deeply the practical nature of the issue studied in this work, we will make a brief presentation of the general principle of operation for a continuous casting equipment:

> *The steel is brought over the installation in a pot from which will flow in the distributor and then in the crystallizer (cast-iron mould from copper - cooled by water circulation). On leaving the crystallizer, solidified front (which surrounds steel that is still liquid) pass in secondary cooling zones, intended to ensure the end of the solidification process.*

The leadership of a continuous casting equipment is based first on a good knowledge of the overall thermal evolution (the thickness of the front solidified at the exit of the crystallizer, the temperature distribution along the body in casting, the amount of heat extracted by each cooling zone, etc.) To develop a continuous casting equipment is motivated mainly by improving the quality of cast steel and by reducing the cost price. Development of numerical methods for calculating the effective solution of some equations that make up the theoretical model is thus essential. The problems of control study may serve to define the optimal strategy for the development of automation on this issue.

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