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AN INVERSE PROBLEM IN THE PHASE-FIELD TRANSITION SYSTEM. THE 2D CASE

Costică Moroşanu

Faculty of Mathematics, "Al. I. Cuza" University of Iaşi, Romania

cmoro@uaic.ro

Abstract The invers problem, denoted by (P), in 2D space dimension governed by the nonlinear parabolic system (the phase-field transition system, introduced by Caginalp [3]), is considered. For every $\varepsilon > 0$, we associate to the nonlinear system an approximating scheme of fractional steps type; corresponding, we consider for (P) the approximating boundary optimal control problem, denoted by (P^ε). On the basis of the convergence of (P^ε) to (P), the necessary optimality conditions are established for (P^ε) and, a conceptual algorithm of gradient type is elaborated in order to compute the sub(optimal) boundary control. The advantage of such approach is that the new method simplifies the numerical computations due to its decoupling feature. The finite element method (**fem**) is used to deduce the discrete equations and numerical results regarding the stability and accuracy of the fractional steps method, as well as the physical aspects (separating zone of solid and liquid states, supercooling, superheating), are reported.

Keywords: boundary value problems for nonlinear parabolic PDE, optimal control, free boundary problem, fractional steps method, finite element method, computer science.

2000 MSC: 35K60, 49, 65, 68, 93.

1. INTRODUCTION

The following nonlinear parabolic system in $Q = [0,T] \times \Omega$, $T > 0$:

$$\begin{cases} \rho V u_t + \dfrac{\ell}{2}\varphi_t = k\Delta u & \text{in } Q, \\ \tau\varphi_t = \xi^2\Delta\varphi + \dfrac{1}{2a}(\varphi - \varphi^3) + 2u & \text{in } Q, \end{cases} \tag{1.1}$$

$$\begin{cases} u(0,x) = u_0(x) & x \in \Omega, \\ \varphi(0,x) = \varphi_0(x) & x \in \Omega, \end{cases} \tag{1.2}$$

$$\begin{cases} \dfrac{\partial u}{\partial \nu} + hu = w(t)g(x) & \text{on } \Sigma = [0,T] \times \partial\Omega, \\ \dfrac{\partial \varphi}{\partial \nu} = 0 & \text{on } \Sigma, \end{cases} \tag{1.3}$$

was proposed by Caginalp [3] to describe the phase transition in a domain $\Omega \subset \mathbb{R}^n$, $n = 1, 2, 3$. System (1.1)–(1.3) is derived from classical Fourier model via Landau-Ginzburg theory. Here u is the reduced temperature, φ is the phase function used

to distinguish between the phases of the material Ω that is involved in the transition process and u_0, $\varphi_0 : \Omega \mapsto \mathbb{R}$, $w : [0,T] \mapsto \mathbb{R}$ are given functions. The positive parameters τ, ξ, ℓ, k, h, a have the following physical meaning: τ is the relaxation time, ξ is the length scale of the interface, ℓ denotes the latent heat, k the heat conductivity, h the heat transfer coefficient and a is an probabilistic measure on the individual atoms, depending on ξ.

The function w in (1.3) represents the temperature of the surrounding at $x \in \partial\Omega$ and it is manipulated by a cooling system according to the equation

$$\begin{cases} w'(t) = \beta w(t) + v(t) & t \in [0,T], \\ w(0) = 0, & . \end{cases} \tag{1.4}$$

where $v \in \mathcal{U}$,

$$\mathcal{U} = \{v(t) \in L^\infty(0,T),\ \ 0 \le v(t) \le R, \quad \text{a.e. } t \in [0,T]\}\,. \tag{1.5}$$

As regards the existence in (1.1)-(1.4), see [7, Proposition 2.1].

Consider that at the moment t the separating region between the phases of the material (solid and liquid, for example) is given by the surface $x = \sigma(t)$ (denoted also by $t = l(x) = \sigma^{-1}(x)$) that is a function of class $C^2(\bar{\Omega}_t)$ such that (see Figure 1)

$$\Omega_t = \{x \in \Omega,\ \ l(x) < t\}$$

is increasing in t, $l(x) = 0$ for all $x \in \Omega_0$, $|\nabla l(x)| \neq 0$ for all $x \in \Omega \setminus \Omega_0$ and $\Delta l(x) > 0$.

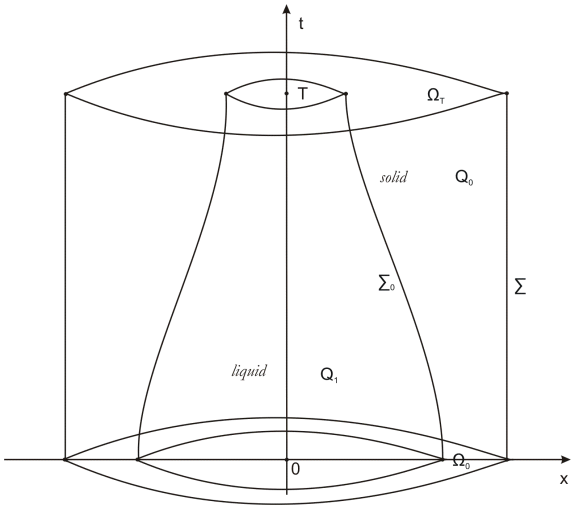

Fig. 1. A material Ω exists in two phases

Let δ and α be two positive constants. We define
solid region: $\{(t,x);\ u(t,x) < -\delta + \alpha,\ |\varphi(t,x) + 1| \le \alpha\}$,

liquid region: $\{(t,x);\ u(t,x) > \delta - \alpha,\ |\varphi(t,x) - 1| \le \alpha\}$,
separating region: $\{(t,x);\ |u(t,x)| \le \delta,\ |\varphi(t,x)| \le \alpha\}$,

and we set

$$\Sigma_0 = \{(t,x) \in Q, \quad t = l(x)\},$$
$$Q_0 = \{(t,x) \in Q, \quad l(x) < t < T\}.$$

The inverse problem that we will study in this paper can be formulated as follows:

Given Σ_0, find the boundary control $w \in L^2(\Sigma)$ such that Q_0 is in the liquid region, $Q_1 = Q \backslash \bar{Q}_0$ is in the solid region and a neighbourhood of Σ_0 is the separating region between the liquid and the solid region.

This inverse problem is in general *"ill posed"* and a common way to treat it is to reformulate it as an optimal control problem with an appropriate cost functional (see [5]). So we will concern in the sequel with an optimal control problem associated to the above inverse problem, namely: we look for $w \in L^2(\Sigma)$ which minimizes the functional

$$(P) \qquad \frac{1}{2}\int_Q [(\varphi+1)^2 + \gamma((u+\delta-\alpha)^-)^2]\chi_{Q_0}\,dxdt + \int_0^T w^2(t)dt,$$

for all (u,φ) solutions of the system (1.1)-(1.4) and for all $v \in \mathcal{U}$. $\gamma > 0$ is a given constant and χ_{Q_0} is the characteristic function of Q_0. In the statement above we have denoted by u^- the negative part of u, i.e.,

$$u^- = -\inf\{u, 0\} = \begin{cases} 0, & \text{if } u > 0; \\ -u, & \text{if } u < 0. \end{cases}$$

2. Approximating optimal control problem

For every $\varepsilon > 0$ we associate to problem (P) the following approximating optimal control problems:

(P^ε) *Minimize*

$$j^\varepsilon(v) = \frac{1}{2}\int_Q [(\varphi^v+1)^2 + \gamma((u^v+\delta-\alpha)^-)^2]\chi_{Q_0}\,dxdt + \int_0^T (w^v)^2(t)dt,$$

on all $(u_\varepsilon, \varphi_\varepsilon, w, v)$ subject to

$$\begin{cases} \rho V u_t^\varepsilon + \dfrac{\ell}{2}\varphi_t^\varepsilon - k\Delta u^\varepsilon = 0 & \text{in} \quad Q_i^\varepsilon = (i\varepsilon,(i+1)\varepsilon)\times\Omega, \\ \dfrac{\partial u^\varepsilon}{\partial \nu} + hu^\varepsilon = w(t) & \text{on} \quad \Sigma_i^\varepsilon = (i\varepsilon,(i+1)\varepsilon)\times\partial\Omega, \\ u^\varepsilon(0,x) = u_0(x) & x \in \Omega, \end{cases} \tag{2.1}$$

$$\begin{cases} w'(t) = \beta w(t) + v(t), \quad t \in [0,T], \\ w(0) = 0, \end{cases} \tag{2.2}$$

$$\begin{cases} \tau\varphi_t^\varepsilon - \xi^2\Delta\varphi^\varepsilon = \dfrac{1}{2a}\varphi^\varepsilon + 2u^\varepsilon \quad \text{in} \quad Q_i^\varepsilon, \\ \dfrac{\partial\varphi_\varepsilon}{\partial\nu} = 0 \qquad\qquad\qquad\quad \text{on} \quad \Sigma_i^\varepsilon, \\ \varphi_+^\varepsilon(i\varepsilon,x) = z(\varepsilon,\varphi_-^\varepsilon(i\varepsilon,x)), \end{cases} \tag{2.3}$$

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

$$\begin{cases} z'(s) + \dfrac{1}{2a}z^3(s) = 0, \qquad s \in [0,T] \\ \\ z(0) = \varphi_-^\varepsilon(i\varepsilon,x)) \qquad \varphi_-^\varepsilon(0,x)) = \varphi_0(x), \end{cases} \tag{2.4}$$

computed at $s = \varepsilon$, for $i = \overline{0, M_\varepsilon - 1}$, with $M_\varepsilon = \left[\frac{T}{\varepsilon}\right]$ and $Q_{M_\varepsilon-1}^\varepsilon = ((M_\varepsilon-1)\varepsilon, T)\times\Omega$. Here $\varphi_+^\varepsilon(i\varepsilon) = \lim\limits_{t\downarrow i\varepsilon}\varphi^\varepsilon(t)$, $\varphi_-^\varepsilon(i\varepsilon) = \lim\limits_{t\uparrow i\varepsilon}\varphi^\varepsilon(t)$.

The convergence of the optimal solution of problem (P^ε) to the optimal solution of problem (P) (as $\varepsilon \to 0$) as well as the necessary optimality conditions in (P^ε), that is:

$$\begin{cases} p_t^\varepsilon + k\Delta p^\varepsilon - \frac{\ell}{\tau}p^\varepsilon + \frac{2}{\tau}q^\varepsilon = 0 \qquad \text{in} \quad Q_i^\varepsilon, \\ \dfrac{\partial p^\varepsilon}{\partial\nu} + hp^\varepsilon = 0 \qquad\qquad\quad \text{on} \quad \Sigma_i^\varepsilon, \\ p_-^\varepsilon((i+1)\varepsilon,x) = 0, \;\; p_-^\varepsilon(T,x) = 0 \quad x \in \Omega, \end{cases} \tag{2.5}$$

$$\begin{cases} \tau q_t^\varepsilon - \dfrac{\ell\xi^2}{2\tau}\Delta p^\varepsilon - \dfrac{\ell}{4a\tau}p^\varepsilon + \dfrac{\xi^2}{\tau}\Delta q^\varepsilon + \dfrac{1}{2a\tau}q^\varepsilon = \varphi^\varepsilon\chi_0 \qquad \text{in} \quad Q_i^\varepsilon, \\ q^\varepsilon = \dfrac{\ell}{2}p^\varepsilon \qquad\qquad\qquad\qquad\qquad\qquad\qquad\quad \text{on} \quad \Sigma_i^\varepsilon, \\ q_-^\varepsilon((i+1)\varepsilon,\cdot) = \exp\Big(\int\limits_0^\varepsilon \frac{3}{2a}(z(t,\cdot)+1)^2dt\Big)q_+^\varepsilon((i+1)\varepsilon,\cdot), \quad \text{on } \Omega, \\ q_-^\varepsilon(T,\cdot) = 0, \end{cases} \tag{2.6}$$

for $i = M_\varepsilon - 2, M_\varepsilon - 3, ..., 1, 0$, where $z(t,\cdot)$ is the solution of (2.4) and

$$v^*(t) = \begin{cases} R, & \text{if } r(t) < 0, \\ 0, & \text{if } r(t) > 0, \end{cases} \tag{2.7}$$

$$r(t) = \int_t^T \Big(\int_{\partial\Omega}(w(s) - kp^\varepsilon(s,x))dx\Big)e^{\beta(s-t)}ds,$$

are proved in [6].

3. Numerical algorithm and results

The aim of this section is to give a numerical algorithm in order to compute the approximating optimal control v^* in problem (P^ε) given by (2.7). In this sense, we have proposed a gradient type method (see [2], [8]).

We assume that $\Omega \subset \mathbb{R}^2$ is a polygonal domain. Let $\varepsilon = T/M$ be the time step size ($M \equiv M_\varepsilon$ in the sequel), let T_r be the triangulation (mesh) over Ω, $\bar{\Omega} = \cup_{K\in T_r} K$ and, let $N_j = (x_k, y_l)$, $j = \overline{1, nn}$, be the nodes associated to T_r. Now, we will construct the discreet form of the problem (P^ε). Using an implicit (backward) finite difference scheme in time and the finite element method in the space, the discrete equations corresponding to (2.1)-(2.3) and (2.5)-(2.6) are, respectively ($i = \overline{1, M}$):

$$\begin{cases} Cu_l^{\varepsilon,i} + \frac{\ell}{2} B\varphi_l^{\varepsilon,i} + \varepsilon khFRu_l^{\varepsilon,i} = B(u^{\varepsilon,i-1} + \frac{\ell}{2}\varphi^{\varepsilon,i-1} + \varepsilon k w^{i-1}\bar{g}_l), \\ D\varphi_l^{\varepsilon,i} - 2\varepsilon B u_l^{\varepsilon,i} = B\cdot(\tau\varphi_l^{\varepsilon,i-1} + \frac{\varepsilon}{2a}), \end{cases} \tag{3.1}$$

$$\begin{cases} Ep_l^{\varepsilon,i} + \varepsilon\frac{2}{\tau} Bq_l^{\varepsilon,i} - \varepsilon khFRp_l^{\varepsilon,i} = Bp_l^{\varepsilon,i+1}, \\ Fq_l^{\varepsilon,i} + Rp_l^{\varepsilon,i} + (\varepsilon h + \varepsilon\frac{\xi^2}{\tau}\frac{\ell}{2})FR\, p_l^{\varepsilon,i} = B(\varphi_l^{\varepsilon,i}\chi_0 + p_l^{\varepsilon,i+1} + q_l^{\varepsilon,i+1}) \end{cases} \tag{3.2}$$

(see [9] for more details).

The conceptual algorithm of gradient type for the calculation of the controller v_ε^* in (2.7) is:

Algorithm CPHT-2D (**C**ontrol **PH**ase **T**ransition-**2D**)

P0. Set *iter:=0*;
Choose $v^{\varepsilon,iter} = (v_0^{\varepsilon,iter}, v_1^{\varepsilon,iter}, ..., v_M^{\varepsilon,iter})$, $v_i^{\varepsilon,iter} \in \mathcal{U}$, $i = \overline{0, M}$;

P1. Compute $w^{\varepsilon,iter} = (w_1^{\varepsilon,iter}, w_2^{\varepsilon,iter}, ..., w_M^{\varepsilon,iter})$ from (1.4);

P2. Compute the approximate matrix

$$u^{\varepsilon,iter} = (u_l^{\varepsilon,1}, ..., u_l^{\varepsilon,M}), \quad \varphi^{\varepsilon,iter} = (\varphi_l^{\varepsilon,1}, ..., \varphi_l^{\varepsilon,M});$$

i.e., for $i = \overline{1, M}$):

- Compute $z(t_i,\cdot) = \pm\dfrac{|\varphi_-^\varepsilon(t_i,\cdot)+1|}{\sqrt{1+\frac{t}{a}(\varphi_-^\varepsilon(t_i,\cdot)+1)^2}} - 1$, on Ω;
- Set $\varphi_+^\varepsilon(t_i,\cdot) = z(t_i,\cdot)$;
- Compute the column vectors $u_l^{\varepsilon,i}$, $\varphi_l^{\varepsilon,i}$, $l = \overline{1, nn}$, solving the linear systems (3.1);

P3. Compute the approximate matrix

$$p^{\varepsilon,iter} = (p_l^{\varepsilon,0}, p_l^{\varepsilon,1}, ..., p_l^{\varepsilon,M-1}), \quad q^{\varepsilon,iter} = (q_l^{\varepsilon,0}, q_l^{\varepsilon,1}, ..., q_l^{\varepsilon,M-1});$$

The column vectors $p_l^{\varepsilon,i}$, $q_l^{\varepsilon,i}$, $i = \overline{0, M-1}$, $l = \overline{1, nn}$,

are obtained solving the linear systems (3.2);

P4. For all $i \in \{0, 1, ..., M\}$ compute $r^{\varepsilon,iter}(t_i)$ and $\tilde{v}^{\varepsilon,iter}(t_i)$, by (2.7);

P5. Compute $\lambda_{iter} \in [0, 1]$ (the steplenght of the gradient method) solution of the minimization process:

$$\min\{j^{\varepsilon}(\lambda v^{\varepsilon,iter} + (1-\lambda)\tilde{v}^{\varepsilon,iter}),\ \ \lambda \in [0,1]\};$$

Set $v^{\varepsilon,iter+1} := \lambda_{iter} v^{\varepsilon,iter} + (1-\lambda_{iter})\tilde{v}^{\varepsilon,iter}$;

P6. (the "*Stopping Criterion*")
if $\|v^{\varepsilon,iter+1} - v^{\varepsilon,iter}\| \leq \eta$
then STOP (the algorithm is convergent)
else $iter := iter + 1$; Go to **P1**.

Let us briefly discuss the main steps in algorithm **CSR-2D**. For approximating the solution of the nonlinear parabolic system (1.1)-(1.4) we have used a numerical method of fractional steps type (see [7], Section 4.2). This method (expressed in step **P2**) avoids the iterative process required by the classical approaches (e.g., Newton's type method) in passing from a time level to another (see [6] for additional details). Moreover, we point out that the equation (2.4) can be solved directly by the separation of variables (the relation (4.7) in [7]). In the above algorithm the variable *iter* represents the number of iterations after which the algorithm **CSR-2D** found the optimal value of the cost functional $j^{\varepsilon}(v)$ in (P^{ε}).

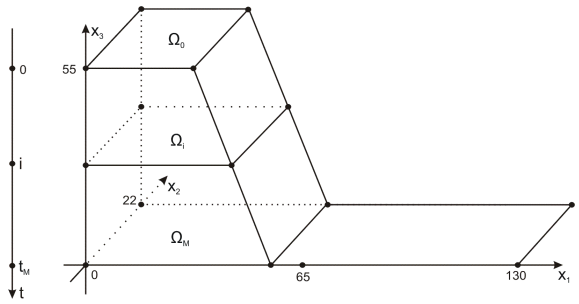

Fig. 2. The domain Q_0

Numerical experiments to compute the boundary control in (P) in 1D was made in the work [5] where an iterative Newton method is used in order to approximate the solution of nonlinear parabolic system (1.1)-(1.4).

In order to test the computer program implementing the algorithm **CPHT-2D**, we have used the following experimental values of parameters:

- the casting speed (V = 12.5 mm/s),

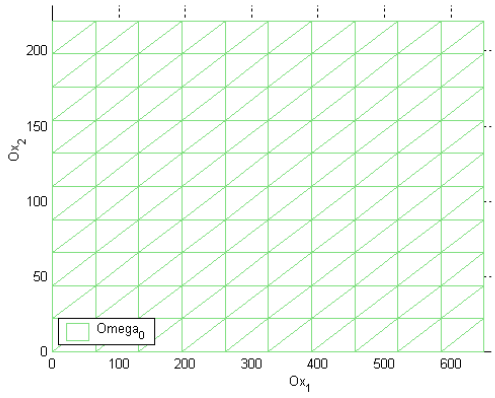

Fig. 3. The triangulation over Ω=[0,650]x[0,220]

- physical parameters: the density (ρ = 7850 kg/m^3), the latent heat ($\ell = 65.28kcal/kg$), the relaxation time ($\tau = 1.0e + 2 * \xi^2$), the length of separating zone ($\xi = .5$), the coefficients of heat transfer ($h = 32.012$), $a = .00008$, $T = 44s$;
- the boundary conditions ($w(t), t \in [0, T]$) in the primary cooling zone:
- dimensions of cristallizer (550 x 1300 x 220), in mm;
- the casting temperature ($u_0 = 1530^0$C);
- the termal conductivity $k(u)$:

  k(u) = [20 100 200 300 400 500 600 700 800 850 900 1000 1100 1200
  1600;1.43e-5 1.42e-5 1.42e-5 1.42e-5 1.42e-5 9.5e-6 9.5e-6 9.5e-6
  8.3e-6 8.3e-6 8.3e-6 7.8e-6 7.8e-6 7.4e-6 7.4e-6].

Figure 2 illustrates the domain Q_0 we have considered in our experiments, while in Figure 3 the number of nodes associated to the mesh in the x_1 and x_2 – axis directions of one half of a rectangular profile is represented. Only a half of the cross-section is used in the computation program.

The *numerical model* (3.1) uses the temperatures $w(t), t \in [0, T]$ measured by the termocouples; corresponding to t_M, the values are ilustrated in the Figure 6 (the line ploted by $*$).

Figures 4 and 5 represents the approximate solution u_M^* for $iter = 1$ and $iter = 5$, respectively. A close examination of them tell us the dimension of the solid and liquid zone resulting by runing the Matlab computation program developed on the basis of the conceptual algorithm **CPHT-2D**.

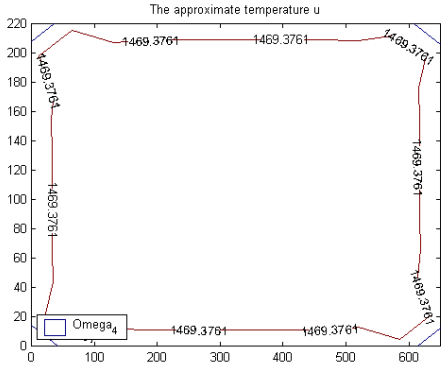

Fig. 4. The approximate temperature u_M^* (*iter*=1)

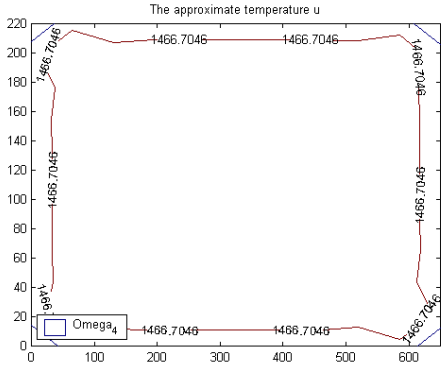

Fig. 5. The approximate temperature u_M^* (*iter*=5)

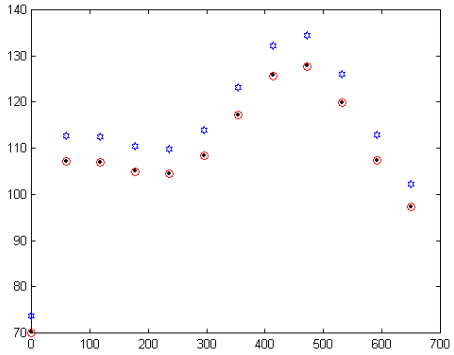

Fig. 6. The boundary optimal control: $*$ - w_M^1, $\bullet$ - w_1^5, $\circ$ - w_M^5

The shape of the graphs in figures 4-5 shows the stability and accuracy of the numerical results obtained by implementing the fractional steps method, but the most interesting aspect that we can observe when analyzing Figure 5, are the presence of *supercooling* and *superheating* phenomenon.

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