An. Şt. Univ. Ovidius Constanţa Vol. 17(1), 2009, 119–136

Fractional steps method to approximate the nonlinear phase-field transition system; 2D case

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Abstract

The phase field transition system (a nonlinear system of parabolic type) introduced by Caginalp [6] to distinguish between the phases of the material that is involved in the solidification process is considered. On the basis of the convergence of an iterative scheme of fractional steps type, a numerical algorithm is constructed in order to approximate the solution of nonlinear parabolic system. The advantage of such approach is that the new method simplifies the numerical computations due to its decoupling feature. The finite element method (**fem**) in 2D is used to deduce the discrete equations and numerical results regarding the physical aspects of solidification process are reported.

1 INTRODUCTION

In this section we will describe the phase-field model introduced in mathematical literature by Caginalp [6]. In this sense we consider a material in a region $\Omega \subset I\!R^N$ $(N = 1, 2, 3)$ which may be in either of two phases, e.g., solid and liquid (see Figure 1). Let us denote by $u(t,x) = \theta(t,x) - \theta_M$, $(t,x) \in [0,T] \times \Omega$, $T \in I\!R_+ = (0,\infty)$, the reduced temperature distribution, where $\theta(t,x)$ represent the temperature of the material and θ_M is the melting temperature (the temperature at which solid and liquid may coexist in equilibrium, separated by a planar interface).

Key Words: Boundary value problems for nonlinear parabolic PDE; Fractional steps method, finite element method.
Mathematics Subject Classification: 35K60, 65.
Received: December, 2008
Accepted: February, 2009

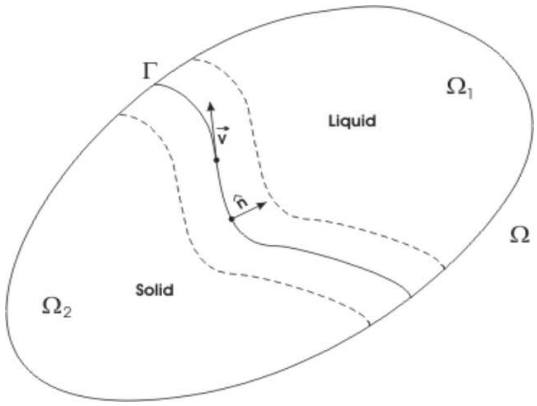

Figure 1. A material Ω exists in two phases. The dotted lines indicate possible thickness of the interface.

1.1 The classical Stefan model in two phases

It is known that in the classical Stefan problem in two phases (the first mathematical model of solidification, see Rubinstein [16]) the *interface* between the solid and liquid (denoted in the sequel by Γ) is considered to be:

$$\Gamma(t) = \{x \in \Omega, \quad u(t,x) = 0\}, \tag{1.1}$$

(what is equivalent with $\theta(t,x) = \theta_M, \quad \forall (t,x) \in \Gamma$) while the liquid and solid regions are defined as:

$$\begin{aligned} \Omega_1(t) &= \{x \in \Omega, \quad u(t,x) > 0\}, \\ \Omega_2(t) &= \{x \in \Omega, \quad u(t,x) < 0\} \end{aligned} \tag{1.2}$$

for all $t \in [0,T]$.

In Ω_1 and Ω_2, the function $u(t,x)$ must then to satisfy the heat diffusion equation

$$u_t = k\Delta u, \tag{1.3}$$

where k is the thermal conductivity divided by heat capacity per unit volume (equal to unity here) assumed to be the same constant in both the phases.

Across the interface Γ (see Figure 1), the latent heat of fusion (per unit mass) ℓ must to be dissipated or to be absorbed, according to conservation law of energy given by:

$$\ell \ \vec{v}(t,x) \cdot \hat{n} \ = \ k(\nabla^+ u(t,x) - \nabla^- u(t,x)) \cdot \hat{n}, \quad x \in \Gamma(t), \tag{1.4}$$

where $\hat{n}$ is the unit normal at each point of $\Gamma(t)$ (in the direction solid $\rightarrow$ liquid), $\vec{v}$ is a local velocity of the interface, and

$$\nabla^+ u(t,x) = \lim_{\bar{x}\to x,\ \bar{x}\in\Omega_1(t)} \nabla u(t,\bar{x}),$$

$$\nabla^- u(t,x) = \lim_{\bar{x}\to x\ \bar{x}\in\Omega_2(t)} \nabla u(t,\bar{x}).$$

Together with the condition

$$u(t,x) = 0 \qquad x \in \Gamma(t), \tag{1.5}$$

(derived from the definition of $\Gamma(t)$) one must specify initial and boundary conditions for $u(t,x)$, e.g.

$$u(t,x) = u_\partial(t,x) \quad x \in \partial\Omega, \quad t > 0, \tag{1.6}$$

$$u(0,x) = u_0(x) \quad x \in \Omega, \tag{1.7}$$

and this complete the mathematical statements of the *classical Stefan model in two phases*. Next, the problem is to find $\Gamma(t)$ and $u(t,x)$ – in suitable function spaces, satisfaing equations (1.3)-(1.7). The interface $\Gamma(t)$ is often called the *free boundary*.

1.2 The phase field transition system

One method for studying the equations (1.3)-(1.7) in the previous subsection is the enthalpy or H-method (Oleinik [14]). The basic idea is to consider the function $H = H(u)$ defined by (ρ, V are physical parameters):

$$H(u) = \rho V u + \tfrac{\ell}{2}\varphi(u), \qquad \varphi(u) = \begin{cases} +1, & u > 0 \\ -1, & u < 0. \end{cases} \tag{1.8}$$

Then the ecuations (1.3)-(1.4) can be incorporate in a weak sense (Oleinik [14]) into the single ecuation:

$$\frac{\partial}{\partial t} H(u) = k\Delta u, \tag{1.9}$$

which represent a balance of heat ecuation.

The physical situation is in generally more complicated than that described by equations (1.3)-(1.4). One of the physical effects neglected by the classical Stefan model is the *surface tension*. If is accepted the Gibbs-Thompson relation

$$u(t,x) = -\frac{\sigma}{\Delta s} \cdot \Xi \qquad (t,x) \in \Gamma(t), \tag{1.10}$$

where σ is the surface tension, Δs is the difference in entropy between solid and liquid, and Ξ is the sum of principal curvatures at a point on the interface, one may consider equations (1.3)-(1.4) together with (1.10) as an alternative to the classical Stefan model. Perhaps the most interesting aspect observed by metallurgists is the presence of liquid at subzero temperatures (the physical phenomena of *supercooling*) and analogously phenomenon for solid (*superheating*). It is clear that the *dual role of the temperature* $u(t,x)$ is no longer possible. Acceptance of the idea that the temperature need not to be zero at the interface (or negative in the solid, etc) leads to the question of how one distinguishes the two phases.

So, let us consider the interface as **a continuous region**, more vast (in which the liquid can coexist with the solid), of finite thickness, in which the change of phase occuring continuously. Then, it is natural that the function φ in (1.8) to be replaced by a function illustrated in Figure 2, i.e., a smooth function with values from $\varphi = -1$ (solid) to $\varphi = +1$ (liquid). **The key question is how one can determine the function** φ ?

In statistical mechanics, a model in which atoms are assumed to interact with a mean field created by the other atoms is known as a *mean field theory*. The Landau-Ginzburg theory of phase transition (see Cahn & Hilliard [7]) is such one theory. Then the free energy of stationary process in this case may be written as

$$F_u(\varphi) = \int_\Omega \Big(\frac{\xi^2}{2} |\nabla \varphi|^2 - \frac{1}{a} G(\varphi) - 2u\varphi \Big) dx \tag{1.11}$$

where ξ is a length scale, $\dfrac{1}{2}|\nabla\varphi|^2$ is an extra term of penalty for φ, $G(\varphi)$ is a symmetric double well potential with minima at ± 1 (for example, $G(\varphi) = \dfrac{1}{8}(\varphi^2 - 1)^2$). The double well potential can be viewed in terms of a probabilistic measure on the individual atoms. The extent with which this measure discriminates against the interfacial region and in favor of the liquid or solid phases, depends on how close a is to zero. The last term in (1.11), which introduces the coupling between u and φ, may be understood as the part of the free energy corresponding to the component u which is altered in time by entropy.

In equilibrium one expects φ to be a minimizer of F_u so that $\delta F_u/\delta\varphi = 0$, i.e. φ verify the equation:

$$\xi^2 \Delta\varphi + \frac{1}{a} g(\varphi) + 2u = 0 \tag{1.12}$$

(the function $g(\varphi)$ is the derivative of the double well potential $G(\varphi)$).

When the material is not in equilibrium (the dependence of time), φ will

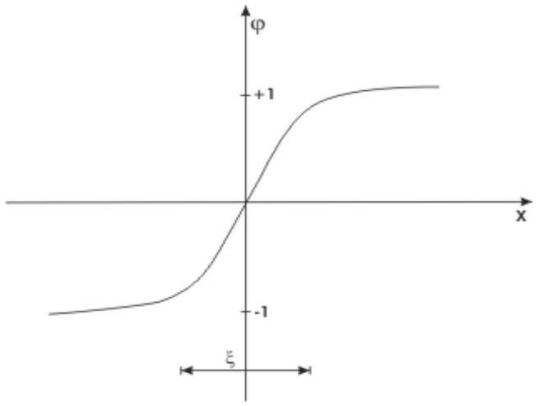

Figure 2. A possible choice of the parameter φ

not minimize $F_u(\varphi)$ but will differ by a term proportional with φ_t. The Euler-Lagrange equations ($\tau\varphi_t = -\delta F_u/\delta\varphi$) then imply the identity:

$$\tau\varphi_t = \xi^2\Delta\varphi + \frac{1}{2a}(\varphi - \varphi^3) + 2u \tag{1.13}$$

(τ is the relaxation time and $g(\varphi) = \frac{1}{2}\varphi(1-\varphi^2)$).

The weak formulation (1.9) (used by Caginalp to introduce a new mathematical model) can be written as:

$$\rho V u_t + \frac{\ell}{2}\varphi_t = k\Delta u. \tag{1.14}$$

Considering now the nonlinear parabolic system derived by unifying the equations (1.13) and (1.14), subject to the initial conditions:

$$u(0,x) = u_0(x) \quad x \in \Omega, \tag{1.15}$$

$$\varphi(0,x) = \varphi_0(x) \quad x \in \Omega \tag{1.16}$$

and appropriate boundary conditions:

$$u = u_\partial(x) \quad x \in \partial\Omega, \tag{1.17}$$

$$\varphi = \varphi_\partial(x) \quad x \in \partial\Omega, \tag{1.18}$$

then, the set of relations (1.13)-(1.18) represents the mathematical model called **phase field transition system** (Caginalp's model).

1.3 The phase field system with a general nonlinearity

Different other nonlinearities $g(\varphi)$ in (1.12), capable to come out the complexity of the physical phenomena (superheating, supercooling, the effect of surface tension, separating zone of liquid and solid states etc) have been proposed by several authors: Bates and Zheng [5], Hoffman and Jiang [8], Moroşanu and Motreanu [12], Penrose and Fife [15], and Liu Xiyuan [17]). The general nonlinear term in Moroşanu and Motreanu [12], $g(x,t,\varphi)$, is (possibly) nonconvex and nonmonotone and cover a large class of nonlinearities, including the known cases as well as other new relevant situations. A main feature of the approach considered there consist in the fact that the double well potential $\int_0^{\varphi} g(\cdot,\cdot,z)dz$ may depend on space and time variables.

The existence and the uniqueness of solution for the phase field system containing a general nonlinearity are established in [12].

1.4 Existence results in phase field system

On $\Sigma = (0,T)\times\partial\Omega$ we can associate to (1.13)-(1.16) different types of boundary conditions, as listed below:

$$\begin{array}{lll}
\partial u/\partial\nu + hu = w(t)g(x) & \varphi = 1, & (BC1)\\
\partial u/\partial\nu + hu = w(t)g(x) & \varphi = 0, & (BC2)\\
\partial u/\partial\nu + hu = 0 & \varphi = 0, & (BC3)\\
u = g_2 & \partial\varphi/\partial\nu = 0, & (BC4)\\
\partial u/\partial\nu + hu = 0 & \partial\varphi/\partial\nu = 0, & (BC5)\\
u = 0 & \varphi = 0, & (BC6)
\end{array}$$

Definition 1.1 By weak solution (u,φ) to (1.13)-(1.16) and (BC1) we mean a pair $(u,\varphi)\in W\times W_0$, $W = L^2(0,T;H^1(\Omega))\cap W^{2,1}([0,T];(H^1(\Omega))')$, $W_0 = L^2(0,T;H_0^1(\Omega))\cap W^{2,1}([0,T];H^{-1}(\Omega))$, which satisfy (1.13)-(1.16) and (BC1) in the following sense

$$\begin{aligned}
&\int\limits_Q(\rho V u_t + \tfrac{\ell}{2}\varphi_t)\psi dxdt + k\int\limits_Q \nabla u\nabla\psi dxdt + kh\int\limits_\Sigma u\psi dxdt\\
&\quad = k\int\limits_\Sigma wg\psi dxdt,
\end{aligned} \tag{1.19}$$

$$\begin{aligned}
&\tau\int\limits_Q\Big(\varphi_t\zeta + \xi^2\nabla\varphi\nabla\zeta\Big)dxdt - \int\limits_Q\tfrac{\tau}{2a}\Big((\varphi-(\varphi+1)^3)\zeta - 2u\zeta\Big)dxdt\\
&\quad = \tfrac{1}{2a}\int\limits_Q\zeta dxdt,
\end{aligned} \tag{1.20}$$

$\forall\,(\psi,\zeta)\in L^2(0,T;H^1(\Omega))\times L^2(0,T;H_0^1(\Omega))$, and

$$u(0,x)=u_0(x),\quad \varphi(0,x)=\varphi_0(x)-1\ \text{ in }\ \Omega. \tag{1.21}$$

Here we have denoted by the same symbol $\int_Q$, the duality between $L^2(0,T;H^1(\Omega))$, $L^2(0,T;(H^1(\Omega))')$ and $L^2(0,T;H_0^1(\Omega))$, $L^2(0,T;H^{-1}(\Omega))$, respectively.

As regards existence in (1.13)-(1.16) and (BC1) we have:

Proposition 1.1 *Assume that* $u_0\in H^1(\Omega)$ *satisfy* $\partial u_0/\partial\nu+hu_0=w(t)g(x)$ *and* $\varphi_0\in L^4(\Omega)\cap H^1(\Omega)$. *If* $w\in W^{1,\infty}(0,T)$, $w(0)=0$, *and* $g\in L^6(\partial\Omega)$, *then the weak solution of* (1.13)-(1.16) *is a strong solution and* $u,\varphi\in W^{1,2}([0,T];L^2(\Omega))\cap L(0,T;H^2(\Omega))$.

In addition, the following estimates holds:

$$\|u\|_{L^2(0,T;H^2(\Omega))}\le C,\quad \|\varphi\|_{L^2(0,T;H^2(\Omega))}\le C,$$

where $C>0$ *depends on* $|\Omega|$, T, ρ, V, τ,k,ℓ,ξ,a,h, $\|u_0\|_{L^2(\Omega)}$, $\|\varphi_0\|_{L^4(\Omega)}$, $\|\nabla u_0\|_{L^2(\Omega)}$, $\|\nabla\varphi_0\|_{L^2(\Omega)}$, $\|w\|_{L^3(0,T)}$, $\|g\|_{L^6(\Gamma)}$ *and* $\max\limits_{y\in\mathbb{R}}\Big\{y^2-\dfrac{1}{4}y^4\Big\}$.

Proof. (see [10]) The proof of Proposition 1.1 in based on some estimates (obtained by using integration by parts, Cauchy's inequality, Holder's inequality, Green's formula and Gronwall's inequality) and on the elliptic regularity of weak solution in [3].

Proposition 1.1 remains true by replacing the boundary condition (BC1) with (BC2), (BC5) or (BC6).

2 FRACTIONAL STEPS METHOD

We shall present now the numerical approximation scheme of fractional steps type in order to compute the solution of nonlinear parabolic system (1.13)-(1.16), assuming different types of boundary conditions.

To fix the idea, consider the system (1.13)-(1.16) and (BC3). For every $\varepsilon\ge 0$ we associate to this problem the following approximating scheme:

$$\begin{aligned}
&\rho V u_t^\varepsilon+\frac{\ell}{2}\varphi_t^\varepsilon-k\Delta u^\varepsilon=0 && \text{in}\quad Q_i^\varepsilon,\\
&\tau\varphi_t^\varepsilon-\xi^2\Delta\varphi^\varepsilon=\frac{1}{2a}\varphi^\varepsilon+2u^\varepsilon && \text{in}\quad Q_i^\varepsilon,\\
&\frac{\partial u^\varepsilon}{\partial\nu}+hu^\varepsilon=0 && \text{on}\quad \Sigma_i^\varepsilon,\\
&\varphi^\varepsilon=0 && \text{on}\quad \Sigma_i^\varepsilon,\\
&\varphi_+^\varepsilon(i\varepsilon)=z(\varepsilon,\varphi_-^\varepsilon(i\varepsilon,x)),
\end{aligned} \tag{2.1}$$

where $Q_i^\varepsilon = (i\varepsilon,(i+1)\varepsilon)\times\Omega$, $\Sigma_i^\varepsilon = (i\varepsilon,(i+1)\varepsilon)\times\partial\Omega$ and $z(t,\varphi_-^\varepsilon(i\varepsilon,x))$ is the solution of

$$\begin{cases} z'(s)+\dfrac{1}{2a}z(s)^3=0 \qquad s\in[i\varepsilon,(i+1)\varepsilon], \\ z(0)=\varphi_-^\varepsilon(i\varepsilon,x); \quad \varphi_-^\varepsilon(0,x)=\varphi_0(x), \end{cases} \tag{2.2}$$

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

2.1 Convergence result

Corresponding to numerical scheme (2.1)-(2.2) we have the following convergence result

Theorem 2.1 *Assume that $u_0,\varphi_0\in W_\infty^1(\Omega)$ satisfying $\partial u_0/\partial\nu+hu_0=0$. Let $(u^\varepsilon,\varphi^\varepsilon)$ be the solution of the approximating scheme* (2.1)-(2.2). *Then, for $\varepsilon\to 0$, one has $(u^\varepsilon(t),\varphi^\varepsilon(t))\to(u^*(t),\varphi^*(t))$ strongly in $L^2(\Omega)$ for any $t\in[0,T]$, where $(u^*,\varphi^*)\in(W^{2,1}([0,T];L^2(\Omega)))^2\cap(L^2(0,T;H^2(\Omega)))^2$ is the weak solution of* (1.13)-(1.16) + (BC3).

Proof. (see [10]) The proof is based on compactness methods. As a matter of fact it turns out from Theorem 2.1 that if $u_0,\varphi_0\in L^2(\Omega)$, then the weak solution $(u^*(t),\varphi^*(t))$ of system (1.13)-(1.16) (see Definition 1.1) is a strong solution, i.e., it is absolutely continuous in t on $[0,T]$ and satisfies a.e. the system (1.13)-(1.16). So Theorem 2.1 can be also viewed as a constructive way to prove the existence in (1.13)-(1.16).

The result in Theorem 2.1 remains true by replacing the boundary condition (BC3) with (BC2) or (BC5).

2.2 Discrete equations in 1D case

Let $\Omega=[0,c]$ be discretized with the grid of $N+1$ equidistant nodes $x_j=jh_1$, $j=0,1,...,N$, where $h_1=c/N$ is the space step size and let the time interval $[0,T]$ be divided into M equal parts with the nodes $t_i=i\varepsilon$, $i=0,1,...,M$, where $\varepsilon=T/M$ is the time step size.

Denote by $(u_j^{\varepsilon,i},\varphi_j^{\varepsilon,i})$ the approximate matrix for $(u^\varepsilon,\varphi^\varepsilon)$ in (2.1)-(2.2)+ (BC5), where $u_j^{\varepsilon,i}=u^\varepsilon(t_i,x_j)$, $\varphi_j^{\varepsilon,i}=\varphi^\varepsilon(t_i,x_j)$, $i=\overline{0,M}$, $j=\overline{0,N}$. Using a standard implicit scheme and a backward-difference formula for (2.1), and the forward-difference formula for (BC5), we obtain:

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}\begin{pmatrix} \bar\varphi^{\varepsilon,i} \\ \bar u^{\varepsilon,i} \end{pmatrix}=\begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \qquad i=1,2,...,M_\varepsilon, \tag{2.3}$$

where

$$\bar{\varphi}^{\varepsilon,i} = (\varphi_0^{\varepsilon,i}, \varphi_1^{\varepsilon,i}, ..., \varphi_N^{\varepsilon,i}) \quad \bar{u}^{\varepsilon,i} = (u_0^{\varepsilon,i}, u_1^{\varepsilon,i}, ..., u_N^{\varepsilon,i}),$$

A_{11}, A_{12}, A_{21}, A_{22} are $(N+1) \times (N+1)$ matrices defined in [9].

The Cauchy problem (2.2) has the solution

$$z(\varepsilon, \varphi_-^{\varepsilon}(i\varepsilon, x)) \;=\; |\varphi_-^{\varepsilon}(i\varepsilon, x)| \sqrt{\frac{a}{a+\varepsilon(\varphi_-^{\varepsilon}(i\varepsilon,x))^2}}, \qquad i = 0, 1, ..., M_\varepsilon - 1. \tag{2.4}$$

Thus, the general algorithm to compute the approximate solution by means of fractional steps method consist in the following sequence (i denotes the time level)

Begin **algfrac_difference**
  $i := 0 \;\rightarrow \bar{\varphi}^{\varepsilon,0}, \bar{u}^{\varepsilon,0}$ from the initial conditions;
  `For` $i := 0$ `to` $M_\varepsilon - 1$ `do`
    Compute $z(\varepsilon, \varphi_-^{\varepsilon}(i\varepsilon, x))$ from (2.4);
    $\bar{\varphi}^{\varepsilon,i} := z(\varepsilon, \varphi_-^{\varepsilon}(i\varepsilon, x))$;
    Compute $\bar{\varphi}^{\varepsilon,i+1}, \bar{u}^{\varepsilon,i+1}$ solving the linear system (2.3);
  `End-for`;
`End`.

A comparison between the fractional steps method and the standard iterative Newton method can be found in [1] and [9].

3 FINITE ELEMENT METHOD

The finite element method (**fem** in short) is a general method for approximating the solution of boundary value problems for partial differential equations. This method derives from the Ritz (or Galerkin) method, characteristic for the finite element method being the chose of the finite dimensional space, namely, the *span* of a set of finite element basis functions.

The steps in solving a boundary value problem using **fem** are:

P0. (D) The direct formulation of the problem;

P1. (V) A variational (weak) formulation for problem (D);

P2. The construction of a finite element mesh (triangulation);

P3. The construction of the finite dimensional space of test function, *called finite element basis functions*;

P4. (V_{nn}) A discrete analogous of (V);

P5. Assembly the linear system of equations;

P6. Solve the system in P5.

3.1 Discrete equations in 2D case

For the sake of simplicity, we will use in the sequel the finite element method only in order to construct the discrete state equations (step **P4**). At the end of section, a numerical algorithm of fractional step type is formulated in order to approximate the weak solution (see Definition 1.1) corresponding to (2.1)+(BC5), that is:

$$\begin{aligned}\left(u_t^\varepsilon + \tfrac{\ell}{2}\varphi_t^\varepsilon, \psi\right) + k(\nabla u^\varepsilon, \nabla\psi) \ + \ kh\int_{\partial\Omega} u^\varepsilon\psi dxdy = 0,\\ \forall\psi \in H^1(\Omega), \text{ a.e. in } (i\varepsilon,(i+1)\varepsilon),\end{aligned} \tag{3.1}$$

$$\begin{aligned}\tau(\varphi_t^\varepsilon, w) + \xi^2(\nabla\varphi^\varepsilon, \nabla w) \ - \ \tfrac{1}{2a}(\varphi^\varepsilon, w) = 2(u^\varepsilon, w),\\ \forall w \in H^1(\Omega), \text{ a.e. in } (i\varepsilon,(i+1)\varepsilon),\end{aligned} \tag{3.2}$$

together with the initial conditions

$$u(0,x) = u_0(x), \quad \varphi(0,x) = \varphi_0(x), \quad x \in \Omega.$$

By $(\cdot,\cdot)$ we have denoted the scalar product in $L^2(\Omega)$.

Let $\varepsilon = T/M$ be the time step size ($M_\varepsilon \equiv M$). We assume that $\Omega \subset \mathbb{R}^2$ is a polygonal domain. Let T_r be the triangulation (mesh) over Ω and $\bar\Omega = \cup_{K\in T_r} K$, and let $N_j = (x_k, y_l), j = \overline{1,nn}$, be the nodes associated to T_r. Denoting by V_{nn} the corresponding finite element space to T_r, then the basic functions $\{b_j\}_{j=1}^{nn}$ of V_{nn} are defined by

$$b_j(N_i) = \delta_{ji}, \quad i,j = \overline{1,nn},$$

and so

$$V_{nn} = span\ \{b_1, b_2, ..., b_{nn}\}.$$

For $i = \overline{1,M}$, we denote by u^i and φ^i the V_{nn} interpolant of u^ε and φ^ε in (3.1)-(3.2), respectively. Then $u^i, \varphi^i \in V_{nn}$ and

$$u^i(x,y) = \sum_{l=1}^{nn} u_l^i b_l(x,y) \quad i = \overline{1,M}, \tag{3.3}$$

$$\varphi^i(x,y) = \sum_{l=1}^{nn} \varphi_l^i b_l(x,y) \quad i = \overline{1,M}, \tag{3.4}$$

where $u_l^i = u^\varepsilon(t_i, N_l)$, $\varphi_l^i = \varphi^\varepsilon(t_i, N_l)$, $i = \overline{1,M}$, $l = \overline{1,nn}$ are the unknowns to be computed.

Using in addition an implicit (backward) finite difference scheme in time, we introduce now the discrete equations corresponding to (3.1)-(3.2) as follows

$$\begin{cases} Ru_l^i + \frac{\ell}{2}B\varphi_l^i + \varepsilon khFRu_l^i &= B(u_l^{i-1} + \frac{\ell}{2}\varphi_l^{i-1}), \\ S\varphi_l^i - 2\varepsilon Bu_l^i = B\tau\varphi_l^{i-1} & \quad i = \overline{1,M} \end{cases} \tag{3.5}$$

where u_l^i and φ_l^i, $l = \overline{1,nn}$, are unknow vectors for time level i.

From the initial conditions (1.15)-(1.16) we have

$$u^0(x,y) \overset{not}{=} u_0(x,y) = \sum_{l=1}^{nn} u_0(N_l)b_l(x,y),$$
$$\varphi^0(x,y) \overset{not}{=} \varphi_0(x,y) = \sum_{l=1}^{nn} \varphi_0(N_l)b_l(x,y),$$

and then (see (3.3)-(3.4))

$$u_l^0 = u_0(N_l), \qquad \varphi_l^0 = \varphi_0(N_l) \qquad l = \overline{1,nn}. \tag{3.6}$$

3.2 The conceptual algorithm

The numerical algorithm to compute the approximate solution by *fractional steps method* can be obtained from the following sequence (again, i denotes the time level)

`Begin` **algfrac_fem**
  $i := 0 \ \rightarrow$ Compute u_l^0, φ_l^0, $l = \overline{1,nn}$ from (3.6)
  `For` $i := 1$ `to` M `do`
    Compute $z_l = z(\cdot, N_l)$, $l = \overline{1,nn}$ from (2.4);
    $\varphi^{i-1} := z_l$, $l = \overline{1,nn}$;
    Compute u_l^i, φ_l^i, $l = \overline{1,nn}$, solving the linear system (3.5);
  `End-for`;
`End`.

The convergence result established by Theorem 2.1, guaranty that the approximate solution $(u^\varepsilon, \varphi^\varepsilon)$, computed by the conceptual algorithm **algfrac_fem** is in fact the approximate solution (u, φ) of nonlinear parabolic system (1.13)-(1.16).

4 NUMERICAL RESULTS

The aim of this section is to present an implementation of conceptual algorithm **algfrac_fem** established in the preview section. The boundary conditions (BC1) we have considered to construct the *numerical model* (3.5). The

application of the *numerical model* requires experimental research and measurements of operational parameters, as well as laboratory research. The most important *input data* in order to do this, are:

- the casting speed ($V = 12.5$ mm/s),
- physical parameters: the density ($\rho = 7850$ 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].

In Figure 3 it can be seen the number of nodes associated to the mesh T_r in the x_1 and x_2 – axis directions of one half of a rectangular profile. Only a half of the cross-section is used in the computation program.

The *numerical model* (3.5) uses the temperatures $w(t), t \in [0, T]$ measured by the termocouples; the values are ilustrated in the Figure 4.

Figures 5-7 represents the approximate solution u^i, φ^i (see (3.3)-(3.4)), corresponding to different moments of time ($ii = 1$, $ii = 5$, $ii = M$).

A close examination of the Figures 5-7 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 **algfrac_fem**.

The shape of the graphs shows the stability and accuracy of the numerical results obtained by implementing the fractional steps method (see [1], [9]), but the most interesting aspect that we can observe analysing the Figure 6-7 are the presence of *supercooling* and *superheating* phenomenon.

5 CONCLUSIONS

Phase field models describe the physical phenomenon of solidification of a liquid in a pure material. They involve two unknowns functions: the temperature of the material and the phase parameter which indicates the liquid

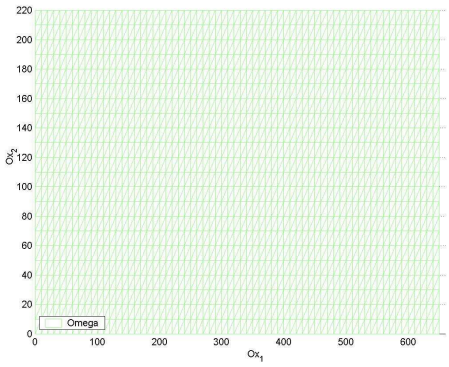

Figure 3. The triangulation T_r over Ω=[0,650]x[0,220]

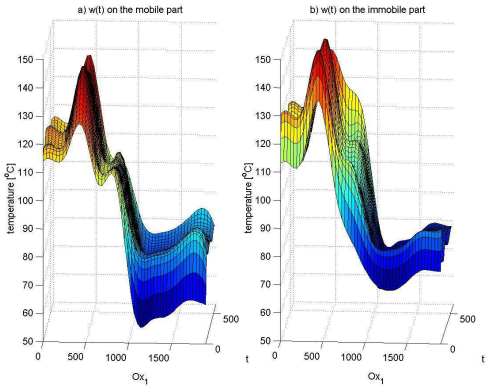

Figure 4. a) the values $w(t)$ on the mobile part, b) the values $w(t)$ on the immobile part

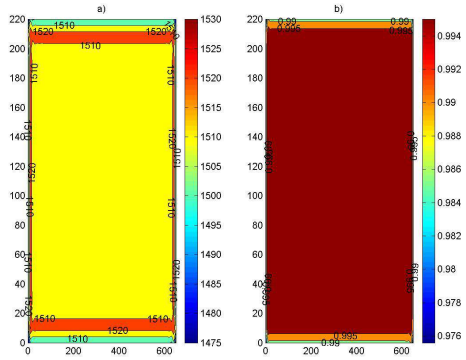

Figure 5. a) the approximate temperature u^1, b) the approximate function φ^1

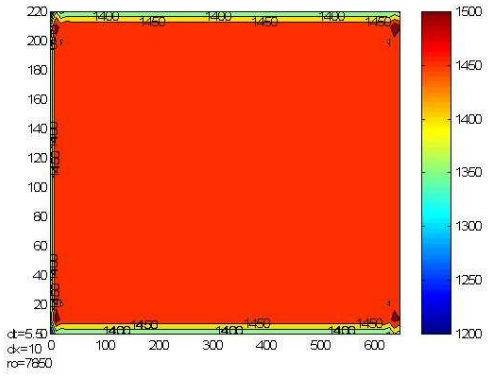

Figure 6. The approximate temperature u^5

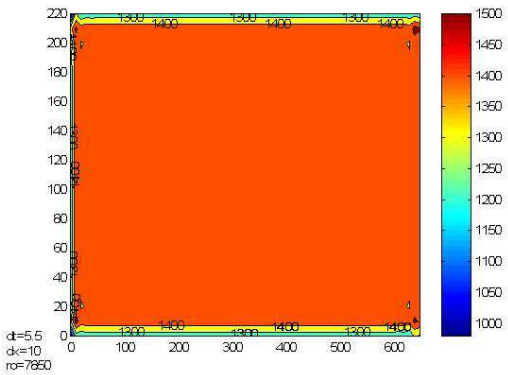

Figure 7. The approximate temperature u^M

or/and solid state of the material. These models can be viewed as extensios of the classical Stefan problem.

The solidification model that we have considered in this paper consist in a system of two nonlinear parabolic differential equations, [6]. This new mathematical description of the real phenomenon reflects more accurately the physical aspects, like: superheating, supercooling, the efects of surface tension, separating zone of solid and liquid states, etc.

From numerical point of view, the main difficulty in treating the phase field transition system is due to the presence of the nonlinear equation corresponding to phase function. Thus it is intensely motivated the work in finding more efficient algorithms in order to compute numerically the solution of such system. A scheme of fractional steps type is considered in this sense. This numerical method avoids the iterative process required by the clasical methods (e.g., Newton's type approaches) in passing from a time level to another. Numerical tests show that the fractional steps method is faster (CPU-time spent is very small) and the stability and accuracy are higher ([1], [9], [11]) than the Newton's methods. The distribution of the temperature and the thickness of the solidifying shell, calculated with the numerical model obtained following this technique, show that it realy is (see Figures 5-7). New fundamental material properties can also be extracted by analisying the implementation of the numerical model (3.5) (see Figure 7).

The numerical solution calculated by this way can be considered as an admissible one for the corresponding optimal control problem, formulated in order to improve, for example, the process optimization of continuous casting.

Generally, the numerical method considered here can be used to approx-

imate the solution of a nonlinear parabolic equation (system) containing a general nonlinear part.

Acknowledgment. The work has been partial elaborated under the support of Contract CEx 05-D11-**84**/28.10.2005, financed by Romanian Ministry of Education and Research.

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