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ON THE NUMERICAL APPROXIMATION OF THE PHASE-FIELD SYSTEM WITH NON-HOMOGENEOUS CAUCHY-NEUMANN BOUNDARY CONDITIONS. CASE 1D

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Abstract A *scheme of fractional steps type*, associated to the nonlinear phase-field transition system in one dimension, is considered in this paper. To approximate the solution of the linear parabolic system introduced by such approximating scheme, we consider three finite differences schemes: **1-IMBDF** (first-order **IM**plicit **B**ackward **D**ifferentiation **F**ormula), **2-IMBDF** (second-order IMBDF) and **2-SBDF** (second-order **S**emi-implicit BDF). A study of stability and the numerical efficiency analysis of this new approach, as well as physical experiments, are performed too.

Keywords: fractional steps method, stability and convergence of numerical methods, computer aspects of numerical algorithms, phase-field transition system, phase changes.
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1. INTRODUCTION

Consider the nonlinear parabolic boundary value problem

$$\begin{cases} \rho c \frac{\partial}{\partial t} u + \frac{\ell}{2} \frac{\partial}{\partial t} \varphi = k \Delta u \\ \tau \frac{\partial}{\partial t} \varphi = \xi^2 \Delta \varphi + \frac{1}{2a}(\varphi - \varphi^3) + 2u \end{cases} \quad \text{in } Q := [0, T] \times \Omega, \tag{1.1}$$

subject to the non-homogeneous Cauchy-Neumann boundary conditions:

$$\begin{cases} \frac{\partial}{\partial \nu} u + hu = w(t, x) \\ \frac{\partial}{\partial \nu} \varphi = 0 \end{cases} \quad \text{on } \Sigma := [0, T] \times \partial\Omega, \tag{1.2}$$

and initial conditions:

$$u(0, x) = u_0(x), \quad \varphi(0, x) = \varphi_0(x) \quad \text{on } \Omega, \tag{1.3}$$

where:

- Ω is a bounded domain in $\boldsymbol{R}$ with smooth boudary $\partial\Omega$,
- $T > 0$ is a given positive number,

- the unknown functions u and φ represent the *reduced temperature distribution* and the *phase function* (used to distinguish between the phases of Ω), respectively,
- $u_0, \varphi_0 : \Omega \to \boldsymbol{R}$ are given functions,
- $w : [0,T] \times \partial\Omega \to \boldsymbol{R}$ also is a given function - *the temperature surrounding at* $\partial\Omega$,
- the positive parameters ρ, c, τ, ξ, ℓ, k, h, a, have the following physical meaning: ρ - is the density, c - is the heat capacity, 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 coeficient and a is an probabilistic measure on the individual atoms (a depends on ξ).

The mathematical model (1.1), introduced by Caginalp [3], has been established in literature as an alternative of the classic two-phase Stefan problem to capture, among others, the effects of *surface tension*, *supercooling*, and *superheating*.

As regards the existence, it is known that under appropiate conditions on u_0, φ_0 and w, the system (1.1)-(1.3) has a unique solution $u, \varphi \in W_p^{2,1}(Q) \cap L^\infty(Q)$, $p > \frac{3}{2}$ (see Morosanu [6]).

Numerical approximation of the phase-field system (1.1) subject to the homogeneous Neumann boundary conditions: $\frac{\partial}{\partial\nu}u + hu = 0$ on Σ, has been analyzed in Morosanu [5]. For other numerical investigation of the phase-field model (subject to various other boundary conditions), see Arnautu & Morosanu [1], Morosanu [4, 6] and references there in.

In order to approximate the above nonlinear problem, a *scheme of fractional steps type* was introduced and analyzed in Benincasa & Morosanu [2], namely, for every $\varepsilon > 0$, it was associated to system (1.1)-(1.3) the following approximating scheme:

$$\begin{cases} \rho c \frac{\partial}{\partial t}u^\varepsilon + \frac{\ell}{2}\frac{\partial}{\partial t}\varphi^\varepsilon = k\Delta u^\varepsilon \\ \tau\frac{\partial}{\partial t}\varphi^\varepsilon = \xi^2\Delta\varphi^\varepsilon + \frac{1}{2a}\varphi^\varepsilon + 2u^\varepsilon \end{cases} \quad \text{in } Q_i^\varepsilon, \tag{1.4}$$

$$\begin{cases} \frac{\partial}{\partial\nu}u^\varepsilon + hu^\varepsilon = w(t,x) \\ \frac{\partial}{\partial\nu}\varphi^\varepsilon = 0 \end{cases} \quad \text{on } \Sigma_i^\varepsilon, \tag{1.5}$$

$$\begin{cases} u^\varepsilon(0,x) = u_0(x) \\ \varphi_+^\varepsilon(i\varepsilon,x) = z(\varepsilon,\ \varphi_-^\varepsilon(i\varepsilon,x)) \end{cases} \quad \text{on } \Omega \tag{1.6}$$

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

$$\begin{cases} z'(s) + \frac{1}{2a}z^3(s) = 0 \quad s \in (0,\varepsilon), \\ z(0) = \varphi_-^\varepsilon(i\varepsilon,x) \quad \varphi_-^\varepsilon(0,x) = \varphi_0(x), \end{cases} \tag{1.7}$$

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

In other words, the fractional steps method consists in decoupling the nonlinear system (1.1)-(1.3) in a linear parabolic system and a nonlinear ordinary differential equation containing the nonlinearity φ^3 of $(1.1)_2$, expressed on a partition of the time interval $[0, T]$ which is composed from M_ε subintervals, the first $M_\varepsilon - 1$ having the same length ε.

The following result establishes the relationship between the solution (u, φ) in (1.1)-(1.3) and the solution $(u^\varepsilon, \varphi^\varepsilon)$ in (1.4)-(1.7).

Theorem 1.1. *Assume that* $u_0, \varphi_0 \in W_\infty^1(\Omega)$ *satisfying* $\frac{\partial}{\partial \nu} u_0 + h u_0 = w(0, x)$, $\frac{\partial}{\partial \nu} \varphi_0 = 0$ *and* $w \in W^1([0, T], L^2(\partial\Omega))$. *Furthermore,* $\Omega \subset \boldsymbol{R}^n$ $(n = 1, 2, 3)$ *is a bounded domain with a smooth boundary. Let* $(u^\varepsilon, \varphi^\varepsilon)$ *be the solution of the approximating scheme* (1.4)-(1.7)*. Then, for* $\varepsilon \to 0$*, one has*

$$(u^\varepsilon(t), \varphi^\varepsilon(t)) \to (u(t), \varphi(t)) \quad \textit{strongly in } L^2(\Omega) \quad \textit{for any } t \in (0, T], \tag{1.8}$$

where $u, \varphi \in W_p^{2,1}([0, T]; L^2(\Omega)) \cap L^2([0, T]; H^2(\Omega))$ *is the solution of the nonlinear system* (1.1)-(1.3).

Based on the result of convergence given by Theorem 1, we will concerned in this work with the numerical approximatin of the solution $(u^\varepsilon, \varphi^\varepsilon)$ of the linear system (1.4)-(1.7).

The rest of paper is organized as follows: in Section 2, for each type of scheme:*1-IMBDF, 2-IMBDF, 2-SBDF*, we have introduced the discrete equations corresponding to (1.4)-(1.7); consequently, conceptual algorithms have been formulated: **Alg_1-IMBDF**, **Alg_2-IMBDF**, **Alg_2-SBDF**, respectively. A stability result for each new approach is stated and proved too. Some physical experiments are reported in the last Section.

2. NUMERICAL METHODS

In this Section we are concerned with the numerical approximation of the solution $(u^\varepsilon, \varphi^\varepsilon)$ in (1.4)-(1.7). As already stated, we will work in one dimension, i.e. $\Delta u^\varepsilon = u_{xx}^\varepsilon$ and $\Delta \varphi^\varepsilon = \varphi_{xx}^\varepsilon$. To fix the ideas, let $\Omega = [0, b] \subset \boldsymbol{R}_+$ and we introduce over it the grid with N equidistant nodes

$$x_j = (j - 1)dx \qquad j = 1, 2, \ldots, N, \;\; dx = b/(N - 1).$$

Given a positive value T and considering $M \equiv M_\varepsilon$ as the number of equidistant nodes in which is divided the time interval $[0, T]$, we set

$$t_i = (i - 1)\varepsilon \qquad i = 1, 2, \ldots, M, \;\; \varepsilon = T/(M - 1).$$

Now we denote by (u^i_j, φ^i_j) the approximate values in the point (t_i, x_j) of the unknown functions $(u^\varepsilon, \varphi^\varepsilon)$. More precisely

$$\begin{array}{l} u^i_j = u^\varepsilon(t_i, x_j) \\ \varphi^i_j = \varphi^\varepsilon(t_i, x_j) \end{array} \qquad i = 1, 2, \ldots, M, \quad j = 1, 2, \ldots, N,$$

or, for later use

$$u^i \overset{\text{not}}{=} \left(u^i_1, u^i_2, \ldots, u^i_N\right)^T \qquad \varphi^i \overset{\text{not}}{=} \left(\varphi^i_1, \varphi^i_2, \ldots, \varphi^i_N\right)^T \qquad i = 1, 2, \ldots, M. \tag{2.1}$$

We continue by explaining how we treat each term in (1.4)-(1.7). The Laplace operator in (1.4) will be approximated by a second order centred finite differences, which means:

$$\begin{array}{l} u^\varepsilon_{xx}(t_i, x_j) = \Delta_{dx} u^i_j \approx \frac{u^i_{j-1} - 2u^i_j + u^i_{j+1}}{dx^2} \\ \varphi^\varepsilon_{xx}(t_i, x_j) = \Delta_{dx} \varphi^i_j \approx \frac{\varphi^i_{j-1} - 2\varphi^i_j + \varphi^i_{j+1}}{dx^2} \end{array} \qquad i = 1, 2, ..., M, \quad j = 1, 2, ..., N, \tag{2.2}$$

(Δ_{dx} is the discrete Laplacian depending on the step-size dx).

From the initial condition $(1.6)_1$, we have

$$u^1_j = u^\varepsilon(t_1, x_j) = u_0(x_j) \quad j = 1, 2, \ldots, N. \tag{2.3}$$

Involving the separation of variables method to solve the Cauchy problem (1.7) (see Morosanu [4]), we get

$$\begin{cases} z(\varepsilon, \varphi^\varepsilon_-(t_1, x)) = z(\varepsilon, \varphi_0(x)) = \varphi_0(x) \sqrt{\frac{a}{a + \varepsilon \varphi_0(x)}}, \\ z(\varepsilon, \varphi^\varepsilon_-(t_i, x)) = \varphi^\varepsilon_-(t_i, x) \sqrt{\frac{a}{a + \varepsilon \varphi^\varepsilon_-(t_i, x)}} \qquad i = 2, ..., M-1. \end{cases} \tag{2.4}$$

Corresponding to Ω, already choosen in one dimension, the boundary $\partial\Omega$ is reduced to the set $\{0, b\}$. Thus the boundary conditions $(1.5)_1$ become

$$\begin{cases} -u_x(0) + h\, u(0) = w(t, 0) \\ u_x(b) + h\, u(b) = w(t, b), \end{cases} \tag{2.5}$$

where the sign in front of $\dfrac{\partial}{\partial \nu} u = u_x$ is $\mp$ because the normal to $[0, b]$ at 0 (b) point in the negative (positive) direction.

Using in (2.5) a farward (backward) finite differences to approximate $u_x(0)$ ($u_x(b)$), we get

$$\begin{cases} -\dfrac{u^i_2 - u^i_1}{dx} + h\, u^i_1 = w^i(0) \\ \dfrac{u^i_N - u^i_{N-1}}{dx} + h\, u^i_N = w^i(b) \end{cases} \qquad i = 1, 2, \ldots, M,$$

i.e.

$$\begin{cases} (1 + dx\, h)u^i_1 - u^i_2 = dx\, w^i(0) \\ -u^i_{N-1} + (1 + dx\, h)u^i_N = dx\, w^i(b) \end{cases} \quad i = 1, 2, \ldots, M, \tag{2.6}$$

where $w^i(0) = w(t_i, 0)$, $w^i(b) = w(t_i, b)$, $i = 1, 2, ..., M$.

To approximate $\varphi_x(0)$ ($\varphi_x(b)$) we will use a backward (forward) finite differences; this leads to

$$\varphi^i_0 = \varphi^i_1, \quad \varphi^i_{N+1} = \varphi^i_N \quad i = 1, 2, \ldots, M, \tag{2.7}$$

where φ^i_0 and φ^i_{N+1} are dummy variables.

For approximating the partial derivative with respect to time, we employed a *first-order scheme* and a *second-order scheme*, namely:

$$\frac{\partial}{\partial t}u^\varepsilon(t_i, x_j) \approx \frac{u^i_j - u^{i-1}_j}{\varepsilon}, \quad \frac{\partial}{\partial t}\varphi^\varepsilon(t_i, x_j) \approx \frac{\varphi^i_j - \varphi^{i-1}_j}{\varepsilon} \tag{2.8}$$

$i = 2, 3, \ldots, M, \quad j = 1, 2, \ldots, N$, and

$$\frac{\partial}{\partial t}u^\varepsilon(t_i, x_j) \approx \frac{3u^i_j - 4u^{i-1}_j + u^{i-2}_j}{2\varepsilon}, \quad \frac{\partial}{\partial t}\varphi^\varepsilon(t_i, x_j) \approx \frac{3\varphi^i_j - 4\varphi^{i-1}_j + \varphi^{i-2}_j}{2\varepsilon} \tag{2.9}$$

$i = 2, 3, \ldots, M, \quad j = 1, 2, \ldots, N$.

Finally we refer to the right hand in (1.4): $\frac{1}{2a}\varphi^\varepsilon(t_i, x_j) + 2u^\varepsilon(t_i, x_j)$. To approximate this quantity (the *reaction term*), will involve two approaches: an implicit and a semi-implicit formula, i.e.:

$$\frac{1}{2a}\varphi^\varepsilon(t_i, x_j) + 2u^\varepsilon(t_i, x_j) \approx \frac{1}{2a}\varphi^i_j + 2u^i_j, \tag{2.10}$$

$i = 1, 2, \ldots, M$, $j = 1, 2, \ldots, N$, and

$$\frac{1}{2a}\varphi^\varepsilon(t_i, x_j) + 2u^\varepsilon(t_i, x_j) \approx 2\left[\frac{1}{2a}\varphi^{i-1}_j + 2u^{i-1}_j\right] - \left[\frac{1}{2a}\varphi^{i-2}_j + 2u^{i-2}_j\right], \tag{2.11}$$

$i = 2, 3, ..., M$, $j = 1, 2, ..., N$ (see Ruuth [7, pp. 156]).

We are now ready to build those three approximation schemes, mentioned at the begining.

A. 1-IMBDF - First-order Implicit Backward Difference Formula. To develop such a scheme, we begin by replacing in (1.4) approximations stated in (2.2), (2.8) and (2.10). We deduce:

$$\begin{cases} \rho c\, \frac{u^i_j - u^{i-1}_j}{\varepsilon} + \frac{\ell}{2}\frac{\varphi^i_j - \varphi^{i-1}_j}{\varepsilon} = k\Delta_{dx}u^i_j \\ \tau\, \frac{\varphi^i_j - \varphi^{i-1}_j}{\varepsilon} = \xi^2\Delta_{dx}\varphi^i_j + \frac{1}{2a}\varphi^i_j + 2u^i_j, \end{cases} \tag{2.12}$$

for $i = 2, 3, \ldots, M$, $j = 1, 2, \ldots, N$.

Using in (2.12) the equalities from (2.2) and arranging convenient, we conclude that, via 1-IMBDF, the system (1.4) is discretized as follows

$$\begin{cases} -k\frac{\varepsilon}{dx^2}u^i_{j-1} + \left[\rho c + 2k\frac{\varepsilon}{dx^2}\right]u^i_j - k\frac{\varepsilon}{dx^2}u^i_{j+1} + \frac{\ell}{2}\varphi^i_j = \rho c u^{i-1}_j + \frac{\ell}{2}\varphi^{i-1}_j \\ -2\varepsilon\, u^i_j - \xi^2\frac{\varepsilon}{dx^2}\varphi^i_{j-1} + \left[\tau + 2\xi^2\frac{\varepsilon}{dx^2} - \frac{\varepsilon}{2a}\right]\varphi^i_j - \xi^2\frac{\varepsilon}{dx^2}\varphi^i_{j+1} = \tau\varphi^{i-1}_j, \end{cases} \tag{2.13}$$

for $i = 2, 3, \ldots, M,\ j = 1, 2, \ldots, N$.

In order to compute the matrix $\begin{pmatrix} u^i_j \\ \varphi^i_j \end{pmatrix}_{i=\overline{2,M},\ j=\overline{1,N}}$, the linear system (2.13) will be solved ascending with respect to time levels. For the first time level ($i = 1$), the values of u^1_j and φ^1_j are computed by (2.3) and (2.4), respectively. Moreover, let us point out from (2.13) and (2.6)-(2.7) that we have $2N$ unknowns for each time-level i, $i = 2, 3, ..., M$ (see also (2.1)).

If, corresponding to $j = 1$ and $j = N$, in $(2.13)_1$ we take $u^i_0 = u^i_1$ and $u^i_{N+1} = u^i_N$, respectively, and if we set

$$\begin{array}{lll} c_1 = -k\frac{\varepsilon}{dx^2} & c_2 = \rho c - 2c_1 & c_3 = \frac{\ell}{2} \\ c_5 = -\xi^2\frac{\varepsilon}{dx^2} & c_6 = \tau - 2c_5 - \frac{\varepsilon}{2a}, & \end{array}$$

than the system (2.13), coupled with (2.6)-(2.7), can be rewritten in matrix form as

$$A\begin{pmatrix} u^i \\ \varphi^i \end{pmatrix} = B\begin{pmatrix} u^{i-1} \\ \varphi^{i-1} \end{pmatrix} + \begin{pmatrix} d^i_1 \\ d^i_2 \end{pmatrix} \qquad i = 2, 3, ..., M, \tag{2.14}$$

where

$$A = \begin{pmatrix} A_{11} & A_{12} \\ -2A_{21} & A_{22} \end{pmatrix} \qquad B = \begin{pmatrix} A_{13} & A_{12} \\ 0 & A_{23} \end{pmatrix}$$

with $A_{11}, A_{12}, A_{13}, A_{21}, A_{22}, A_{23}$ having the same size $N \times N$, and

$$A_{11} = \begin{pmatrix} a_1 & c_1 - 1 & 0 & \cdots & 0 & 0 & 0 \\ c_1 & c_2 & c_1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & c_1 & c_2 & c_1 \\ 0 & 0 & 0 & \cdots & 0 & c_1 - 1 & a_1 \end{pmatrix}$$

$a_1 = c_1 + c_2 + 1 + dx \cdot h,$

$$A_{22} = \begin{pmatrix} c_5 + c_6 & c_5 & 0 & \cdots & 0 & 0 & 0 \\ c_5 & c_6 & c_5 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & c_5 & c_6 & c_5 \\ 0 & 0 & 0 & \cdots & 0 & c_5 & c_5 + c_6 \end{pmatrix}$$

$$A_{12} = \begin{pmatrix} c_3 & 0 & \cdots & 0 & 0 \\ 0 & c_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & c_3 & 0 \\ 0 & 0 & \cdots & 0 & c_3 \end{pmatrix} \quad A_{21} = \begin{pmatrix} dt & 0 & \cdots & 0 & 0 \\ 0 & dt & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & dt & 0 \\ 0 & 0 & \cdots & 0 & dt \end{pmatrix}$$

$$A_{13} = \begin{pmatrix} \rho c & 0 & \cdots & 0 & 0 \\ 0 & \rho c & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & \rho c & 0 \\ 0 & 0 & \cdots & 0 & \rho c \end{pmatrix} \quad A_{23} = \begin{pmatrix} \tau & 0 & \cdots & 0 & 0 \\ 0 & \tau & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & \tau & 0 \\ 0 & 0 & \cdots & 0 & \tau \end{pmatrix}$$

$$d_1^i = \begin{pmatrix} dx \cdot w^i(0) \\ 0 \\ \vdots \\ 0 \\ dx \cdot w^i(b) \end{pmatrix} \quad d_2^i = \begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix}.$$

Therefore, the general design of the algorithm to calculate the approximate solution of nonlinear system (1.1)-(1.3), via *fractional steps method* and *1-IMBDF*, is the following one

```
Begin Alg_1-IMBDF
    Choose T > 0, b > 0;
    Choose M > 0, N > 0 and compute ε, dx;
    Choose u_0, φ_0, w;
    i := 1 → u^1 from the initial conditions (2.3);
    For i = 2 to M do
        Compute φ^{i-1} = z(ε, φ_-^ε(t_{i-1}, ·)) using (1.6)_2 and (2.4);
        Compute u^i, φ^i solving the linear system (2.14);
    End-for;
End.
```

B. 2-IMBDF - Second-order Implicit Backward Difference Formula. To solve the system (1.4) we consider now a *second-order implicit scheme*, i.e.:

$$\begin{cases} \rho c \, \frac{3u_j^i - 4u_j^{i-1} + u_j^{i-2}}{2\varepsilon} + \frac{\ell}{2} \frac{3\varphi_j^i - 4\varphi_j^{i-1} + \varphi_j^{i-2}}{2\varepsilon} = k\Delta_{dx} u_j^i \\ \tau \, \frac{3\varphi_j^i - 4\varphi_j^{i-1} + \varphi_j^{i-2}}{2\varepsilon} = \xi^2 \Delta_{dx} \varphi_j^i + \frac{1}{2a} \varphi_j^i + 2u_j^i, \end{cases} \tag{2.15}$$

for $i = 2, 3 \ldots, M$, $j = 1, 2, \ldots, N$, and u^0, φ^0 considered as dummy variables.

Following the same schedule as above, we conclude that, via *2-IMBDF*, the system (1.4) is discretized as follows:

$$\left\{\begin{array}{l} 2c_1u^i_{j-1} + \left(3\rho c + 4k\frac{\varepsilon}{dx^2}\right)u^i_j + 2c_1u^i_{j+1} + 3c_3\varphi^i_j \\ \qquad = \rho c\left(4u^{i-1}_j - u^{i-2}_j\right) + c_3\left(4\varphi^{i-1}_j - \varphi^{i-2}_j\right), \\ -4\varepsilon\, u^i_j + 2c_5\varphi^i_{j-1} + \left(3\tau - 4c_5 - \frac{\varepsilon}{a}\right)\varphi^i_j \\ \qquad\qquad +2c_5\varphi^i_{j+1} = \tau\left(4\varphi^{i-1}_j - \varphi^{i-2}_j\right), \end{array}\right. \tag{2.16}$$

for $i = 2, 3, \ldots, M,\ j = 1, 2, \ldots, N$.

Remembering the same considerations (developed at begining of Section) with respect to: *initial conditions* - relations (2.3)-(2.4), *boundary conditions* - relations (2.6)-(2.7), *unknown vector* for each time-level i - which was denoted by u^i and φ^i, and setting

$$c_7 = 3\rho c + 4k\frac{\varepsilon}{dx^2} \quad c_8 = 3\tau - 4c_5 - \frac{\varepsilon}{a},$$

the system (2.16) can be written as a matrix equation,

$$E\begin{pmatrix} u^i \\ \varphi^i \end{pmatrix} = 4B\begin{pmatrix} u^{i-1} \\ \varphi^{i-1} \end{pmatrix} - B\begin{pmatrix} u^{i-2} \\ \varphi^{i-2} \end{pmatrix} + \begin{pmatrix} d^i_1 \\ d^i_2 \end{pmatrix} \quad i = 2, 3, ..., M, \tag{2.17}$$

where

$$E = \begin{pmatrix} E_{11} & 3A_{12} \\ -4A_{21} & E_{22} \end{pmatrix}$$

with E_{11}, E_{22} having the same size $N \times N$, and

$$E_{11} = \begin{pmatrix} e_1 & 2c_1 - 1 & 0 & \cdots & 0 & 0 & 0 \\ 2c_1 & c_7 & 2c_1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2c_1 & c_7 & 2c_1 \\ 0 & 0 & 0 & \cdots & 0 & 2c_1 - 1 & e_1 \end{pmatrix}$$

$e_1 = 2c_1 + c_7 + 1 + dx \cdot h$,

$$E_{22} = \begin{pmatrix} 2c_5 + c_8 & 2c_5 & 0 & \cdots & 0 & 0 & 0 \\ 2c_5 & c_8 & 2c_5 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2c_5 & c_8 & 2c_5 \\ 0 & 0 & 0 & \cdots & 0 & 2c_5 & 2c_5 + c_8 \end{pmatrix}.$$

Summing up, we can conclude that the general design of the algorithm to calculate the approximate solution of nonlinear system (1.1)-(1.3), via *fractional steps method* and *2-IMBDF*, is the following one

```
Begin Alg_2-IMBDF
    Choose T > 0, b > 0;
    Choose M > 0, N > 0 and compute ε, dx;
    Choose u_0, φ_0, w;
    i := 1 → u^1 from the initial conditions (2.3);
            φ^1 = z(ε, φ^ε_(t_1, ·)) from (2.4)_1;
    i := 0 → u^0 = u^1, φ^0 = φ^1;
    For i = 2 to M do
        Compute φ^{i−1} = z(ε, φ^ε_(t_{i−1}, ·)) using (1.6)_2 and (2.4);
        Compute u^i, φ^i solving the linear system (2.17);
    End-for;
End.
```

C. 2-SBDF - Second-order Semi-implicit Backward Difference Formula. The purpose of this Subsection is to implement a *2-SBDF* method to approximate the solution $(u^\varepsilon, \varphi^\varepsilon)$ in (1.4)-(1.7). The work is based especially on relations (2.9) and (2.11). Consequently, replacing in (1.4) the approximations mentioned above, we deduce the following system of equations:

$$\begin{cases} \rho c\, \frac{3u_j^i - 4u_j^{i-1} + u_j^{i-2}}{2\varepsilon} + \frac{\ell}{2}\frac{3\varphi_j^i - 4\varphi_j^{i-1} + \varphi_j^{i-2}}{2\varepsilon} = k\Delta_{dx} u_j^i \\ \tau\, \frac{3\varphi_j^i - 4\varphi_j^{i-1} + \varphi_j^{i-2}}{2\varepsilon} = \xi^2 \Delta_{dx}\varphi_j^i + 2\left[\frac{1}{2a}\varphi_j^{i-1} + 2u_j^{i-1}\right] - \left[\frac{1}{2a}\varphi_j^{i-2} + 2u_j^{i-2}\right] \end{cases} \tag{2.18}$$

$i = 2, 3, ..., M,\ j = 1, 2, ..., N$, where, following the same strategy as in previous Subsection, we obtain the discrete system (see also (2.16)):

$$\begin{cases} 2c_1 u_{j-1}^i + c_7 u_j^i + 2c_1 u_{j+1}^i + 3c_3 \varphi_j^i \\ \quad = \rho c\left(4u_j^{i-1} - u_j^{i-2}\right) + c_3\left(4\varphi_j^{i-1} - \varphi_j^{i-2}\right), \\ 2c_5 \varphi_{j-1}^i + (3\tau - 4c_5)\,\varphi_j^i + 2c_5 \varphi_{j+1}^i \\ \quad = 8\varepsilon\, u_j^{i-1} + \left(4\tau + \frac{2\varepsilon}{a}\right)\varphi_j^{i-1} - 4\varepsilon\, u_j^{i-2} - \left(\tau + \frac{\varepsilon}{a}\right)\varphi_j^{i-2}, \end{cases} \tag{2.19}$$

$i = 2, 3, \ldots, M,\ j = 1, 2, \ldots, N$.

Setting

$$c_9 = 3\tau - 4c_5 \quad c_{10} = 4\tau + 2\frac{\varepsilon}{a} \quad c_{11} = \tau + \frac{\varepsilon}{a},$$

the system (2.19) can be rewritten in matrix form as

$$X\!\left(\begin{array}{c} u^i \\ \varphi^i \end{array}\right) = Y\left(\begin{array}{c} u^{i-1} \\ \varphi^{i-1} \end{array}\right) - Z\left(\begin{array}{c} u^{i-2} \\ \varphi^{i-2} \end{array}\right) + \left(\begin{array}{c} d_1^i \\ d_2^i \end{array}\right) \quad i = 2, 3, ..., M, \tag{2.20}$$

where

$$X = \left(\begin{array}{cc} E_{11} & 3A_{12} \\ 0 & X_{22} \end{array}\right) \quad Y = \left(\begin{array}{cc} 4A_{13} & 4A_{12} \\ 8A_{21} & Y_{22} \end{array}\right) \quad Z = \left(\begin{array}{cc} A_{13} & A_{12} \\ 4A_{21} & Z_{22} \end{array}\right)$$

with $A_{12}, X_{22}, A_{13}, A_{21}, Y_{22}, Z_{22}$ having the same size $N \times N$, and

$$X_{22} = \begin{pmatrix} 2c_5 + c_9 & 2c_5 & 0 & \cdots & 0 & 0 & 0 \\ 2c_5 & c_9 & 2c_5 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2c_5 & c_9 & 2c_5 \\ 0 & 0 & 0 & \cdots & 0 & 2c_5 & 2c_5 + c_9 \end{pmatrix},$$

$$Y_{22} = \begin{pmatrix} c_{10} & 0 & \cdots & 0 & 0 \\ 0 & c_{10} & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & c_{10} & 0 \\ 0 & 0 & \cdots & 0 & c_{10} \end{pmatrix}, \quad Z_{22} = \begin{pmatrix} c_{11} & 0 & \cdots & 0 & 0 \\ 0 & c_{11} & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & c_{11} & 0 \\ 0 & 0 & \cdots & 0 & c_{11} \end{pmatrix}.$$

Summing up, we can conclude that the general design of the algorithm to calculate the approximate solution of nonlinear system (1.1)-(1.3) by *fractional steps scheme* via *2-SBDF method* is the following one

Begin **Alg_2-SBDF**
  Choose $T > 0$, $b > 0$;
  Choose $M > 0$, $N > 0$ and compute ε, dx;
  Choose u_0, φ_0, w;
  $i := 1 \to u^1$ from the initial conditions (2.3);
    $\varphi^1 = z(\varepsilon, \varphi^\varepsilon_-(t_1, \cdot))$ from $(2.4)_1$;
  $i := 0 \to u^0 = u^1, \varphi^0 = \varphi^1$;
  For $i = 2$ to M do
    Compute $\varphi^{i-1} = z(\varepsilon, \varphi^\varepsilon_-(t_{i-1}, \cdot))$ using $(1.6)_2$ and (2.4);
    Compute u^i, φ^i solving the linear system (2.20);
  End-for;
End.

As it is well known, most initial value problems reduce to solving large sparse linear systems of the form (2.14), (2.17) or (2.20). For later use (e.g., numerical implementation of conceptual algorithms), we will proof the following

Lemma 2.1. *If*

$$\tau + \xi^2 \frac{\varepsilon}{dx^2} \neq \frac{\varepsilon}{2a}, \tag{2.21}$$

then the matrix coefficients in linear system (2.14) *can be factored into the product of a lower-triangular matrix and an upper-triangular matrix* (*LU - factorization*).

Proof. Let denote by a_{mn}, $m, n = 1, 2, \cdots, 2N$, the elements of matrix coefficients in linear system (2.14). Analyzing the main diagonal elements of block matrices A_{11} and A_{22} in (2.14), first we finding that $a_1 = c_1 + c_2 + 1 + dx \cdot h = \rho c + k \frac{\varepsilon}{dx^2} + 1 + dx \cdot h \neq 0$

and $c_2 = \rho c - 2c_1 = \rho c + 2k\frac{\varepsilon}{dx^2} \neq 0$. Observing now that $c_5 + c_6 \neq 0$ reflect the assumptions expressed in (2.21), as well as that $c_6 \neq 0$, we find easily that $a_{mm} \neq 0$ $\forall m = 1, 2, \cdots, 2N$. So Gaussian elimination can be performed on the system (2.14) without interchanges; consequently A has an LU factorization. ∎

Remark 2.1. *i. if*

$$\tau + \xi^2 \frac{\varepsilon}{dx^2} \neq \frac{\varepsilon}{2a},$$

then the matrix coefficients E in linear system (2.17) *has a LU factorization;*

ii. always, the matrix coefficients X in linear system (2.20) *has a LU factorization.*

3. STABILITY CONDITIONS

To establish conditions of stability for the linear difference equations (2.14), (2.17) and (2.20) introduced in the previous section, we will use in our analysis the Lax-Richtmyer definition of stability, expressed in terms of norm $\|\cdot\|_\infty$ (see Smith [8], pp. 48). To fixed the ideas, we will focus our atention on equation (2.14). This may be rewritten in a more convenient form as

$$\begin{pmatrix} u^i \\ varphi^i \end{pmatrix} = A^{-1}B \begin{pmatrix} u^{i-1} \\ \varphi^{i-1} \end{pmatrix} + A^{-1} \begin{pmatrix} d_1^i \\ d_2^i \end{pmatrix} \quad i = 2, 3, ..., M \tag{3.1}$$

(the existence of A^{-1} will be proved in the proof of Proposition 3.1 below). In addition, the matrix A can be written in the form

$$A = D(I + D^{-1}G) \tag{3.2}$$

where $D = diag(a_1, c_2, \cdots, c_2, a_1, c_5 + c_6, c_6, \cdots, c_6, c_5 + c_6)$ and $G = A - D$. Thus, noting $a_2 = c_5 + c_6$, we have

$$D^{-1}G = \begin{pmatrix}
0 & \frac{c_1-1}{a_1} & 0 & \cdots & 0 & 0 & \frac{c_3}{a_1} & 0 & 0 & \cdots & 0 & 0 & 0 \\
\frac{c_1}{c_2} & 0 & \frac{c_1}{c_2} & \cdots & 0 & 0 & 0 & \frac{c_3}{c_2} & 0 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 0 & \frac{c_1}{c_2} & 0 & 0 & 0 & \cdots & 0 & \frac{c_3}{c_2} & 0 \\
0 & 0 & 0 & \cdots & \frac{c_1-1}{a_1} & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & \frac{c_3}{a_1} \\
-\frac{2\varepsilon}{a_2} & 0 & 0 & \cdots & 0 & 0 & 0 & \frac{c_5}{a_2} & 0 & \cdots & 0 & 0 & 0 \\
0 & -\frac{2\varepsilon}{c_6} & 0 & \cdots & 0 & 0 & \frac{c_5}{c_6} & 0 & \frac{c_5}{c_6} & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & -\frac{2\varepsilon}{c_6} & 0 & 0 & 0 & 0 & \cdots & \frac{c_5}{c_6} & 0 & \frac{c_5}{c_6} \\
0 & 0 & 0 & \cdots & 0 & -\frac{2\varepsilon}{a_2} & 0 & 0 & 0 & \cdots & 0 & \frac{c_5}{a_2} & 0
\end{pmatrix}$$

and a simple analysis of all lines in matrix $D^{-1}G$ allows us to deduce that we only have four distinct lines. The sum of each such line is written in vector v below (recall that $a_1 = c_1 + c_2 + 1 + dx \cdot h$ and $a_2 = c_5 + c_6$)

$$v = \left[\frac{c_1 + c_3 - 1}{a_1}, \frac{2c_1 + c_3}{c_2}, \frac{-2\varepsilon + c_5}{a_2}, \frac{-2\varepsilon + 2c_5}{c_6}\right]. \tag{3.3}$$

Let's denote by

$v_{max} = \max\{|c_1 + c_3 - 1|, |2c_1 + c_3|, |-2\varepsilon + c_5|, |-2\varepsilon + 2c_5|\}$,

and

$v_{min} = \min\{|c_1 + c_2 + 1 + dx \cdot h|, |c_2|, |a_2|, |c_6|\}$.

Now we are able to prove the following result with respect to the stability in matrix equation (3.1).

Proposition 3.1. *Suppose that $v_{min} - v_{max} > 0$. If one of the following conditions is true:*

i) $\rho c + \frac{\ell}{2} > \tau$ & $\dfrac{\rho c + \frac{\ell}{2}}{v_{min} - v_{max}} < 1$

or

ii) $\rho c + \frac{\ell}{2} \leq \tau$ & $\dfrac{\tau}{v_{min} - v_{max}} < 1$,

then the equation (3.1) *is stable. Otherwise, it is unstable.*

Proof. The proof is reduced to checking the condition of stability which, based on the Lax-Richtmyer definition mentioned above and taking into account the relation (3.1), it reduces to check the inequality

$$\|A^{-1}B\|_\infty < 1.$$

We begin our analyse by determining an estimate for $\|D^{-1}G\|_\infty$. As we have already noted (see relation (3.3)), this is equivalent with the following equality: $\|D^{-1}G\|_\infty = \max|v|$, wherefrom we easily derive the estimate

$$\|D^{-1}G\|_\infty < \frac{v_{max}}{v_{min}}. \tag{3.4}$$

The estimate (3.4) allows us now to prove the existence of A^{-1}. Indeed, since by hypothesis we have assumed that $v_{max} < v_{min}$ than $\|D^{-1}G\|_\infty < 1$ which guarantees that there exist $(I + D^{-1}G)^{-1}$. Moreover, there exist A^{-1} and $A^{-1} = (I + D^{-1}G)^{-1}D^{-1}$. Using the well known inequality: $\|(I + D^{-1}G)^{-1}\|_\infty \leq \frac{1}{1 - \|D^{-1}G\|_\infty}$ and making use of (3.2), it follows that

$$\|A^{-1}\|_\infty \leq \|(I + D^{-1}G)^{-1}\|_\infty \|D^{-1}\|_\infty \leq \frac{1}{1 - \|D^{-1}G\|_\infty}\|D^{-1}\|_\infty. \tag{3.5}$$

How $\|D^{-1}G\|_\infty \leq 1$ imply that $1 - \|D^{-1}G\|_\infty \geq 1 - \frac{v_{max}}{v_{min}} > 0$, we easily deduce from this that

$$0 < \frac{1}{1 - \|D^{-1}G\|_\infty} \leq \frac{v_{min}}{v_{min} - v_{max}}.$$

Since $||D^{-1}||_\infty \leq \frac{1}{v_{min}}$ and involving the above estimate, from (3.5) we finaly obtain

$$||A^{-1}||_\infty < \frac{1}{v_{min} - v_{max}}. \tag{3.6}$$

Now we turn our attention to matrix B. Analyzing the matrix B lines, it follows that

$$||B||_\infty = \max\left\{\rho c + \frac{\ell}{2}, \tau\right\}. \tag{3.7}$$

Summing up and making use of (3.6)-(3.7) we derive the following estimate

$$||A^{-1}B||_\infty \leq ||A^{-1}||_\infty ||B||_\infty < \frac{1}{v_{min} - v_{max}} ||B||_\infty,$$

which, in either cases i) or ii) leads us to the estimate $||A^{-1}B||_\infty < 1$ as we claimed at begining of proof. ∎

Remark 3.1. *Concerning the stability of the linear system* (2.17) *we can finding easily that the conditions* i), ii) *in* Proposition 3.1 *are kept and,*

$v_{max} = \max\{|2c_1 + 3c_3 - 1|, |2c_1 + 3c_3|, |-4\varepsilon + 2c_5|, |-4\varepsilon + 4c_5|\},$

$v_{min} = \min\{|2c_1 + c_7 + 1 + dx \cdot h|, |c_7|, |2c_5 + c_8|, |c_8|\},$

while, for the linear system (2.20) *the parameter* τ *in conditions* i), ii) - Proposition 3.1*, must be replaced with* $2\varepsilon + \tau + \frac{\varepsilon}{2a}$ *and,*

$v_{max} = \max\{|2c_1 + 3c_3 - 1|, |2c_1 + 3c_3|, |2c_5|, |4c_5|\},$

$v_{min} = \min\{|2c_1 + c_7 + 1 + dx \cdot h|, |c_7|, |2c_5 + c_9|, |c_9|\}.$

4. NUMERICAL EXPERIMENTS

The aim of this Section is to present numerical experiments implementing the conceptual algorithms **Alg_1-IMBDF**, **Alg_2-IMBDF** and **Alg_2-SBDF**. Corresponding to input data T, b, M, N, we have used several different values while, for the model's parameters we have considered industrial values, which are:

- the casting speed (c = 12.5 mm/s),
- physical parameters:
  - the density (ρ = 7.85 kg/m^3),
  - the latent heat ($\ell = 65.28\ kcal/kg$),
  - the termal conductivity ($k = 7.8e - 2$),
  - the length of separating zone (ξ = .5),
  - the relaxation time ($\tau = 1.0e + 3 * \xi^2$),

- the coefficients of heat transfer ($h = 32.012$),
- $a = \sqrt{\xi}$;

The initial values $\varphi_0(x_j)$, $j = 1, 2, ..., N$, ploted in Figure 4.1 - left side, were computed via Matlab function `csapi(fi0)` - cubic spline interpolant to the given data:

```
fi0=[-1.4 -1.4 -1.44 -1.42 -1.42 -1.44 -1.43 -1.43 -1.42 -1.42 -1.4 -1.4 -1.25 -1.2 -1.17 -1.15 ...
-1.1 -1.08 -1.0 -.95 -.9 -.85 -.88 -.6 .0 .5 -.92 -.25 .8 -.7 .58 .75 .58 -.63 -.59 .69 -.72 .7 -.59 -.5 ...
.7 -.79 -.87 -.88 .0 .72 -.8 .81 .0 -.89 .0 .7 .55 .68 -.49 .79 .0 -.1 -.8 -.78 -.83 .69 -.8 .68 .5 .7 ...
.59 1. 1.08 1.1 1.15 1.17 1.2 1.25 1.3 1.3 1.25 1.24 1.3 1.31 1.3 1.32 1.3 1.3];
```

The initial values $u_0(x_j)$, $j = 1, 2, ..., N$, ploted in Figure 1 - right side, were computed as solution of the discrete form to the stationary equation $(2a)^{-1}[\varphi_0(x) - \varphi_0^3(x)] + 2u_0(x) = 0$ (see Caginalp [3]), i.e.:

$$(2a)^{-1}[\varphi_0(x_j) - (\varphi_0(x_j)^3)] + 2u_0(x_j) = 0 \quad j = 1, 2, ..., N.$$

Now (see $(2.4)_1$) we are able to calculate the vector $\left(z\left(\varepsilon, \varphi_0(x_j)\right)\right)_{j=\overline{1,N}}$, ploted in Figure 2, and the vectors: $\varphi^1 = \left(\varphi_j^1\right)_{j=\overline{1,N}}$ and $u^1 = \left(u_j^1\right)_{j=\overline{1,N}}$ (see relations (2.3), $(1.6)_2$ and (2.4)). As the schemes 2-IMBDF and 2-SBDF involves three time levels, we consider at the first time level $i := 0$ the values $u^0 = u^1$ and $\varphi^0 = \varphi^1$. Consequently, the right side of the linear systems (2.17) and (2.20), corresponding to the first iteration of the cycle "`for`" in algorithms **Alg_2-IMBDF** and **Alg_2-SBDF** ($i = 2$), become:

$3B\begin{pmatrix} u^1 \\ \varphi^1 \end{pmatrix} + \begin{pmatrix} d_1^2 \\ d_2^2 \end{pmatrix}$ and $\begin{pmatrix} 3A_{13} & 3A_{12} \\ 4A_{21} & Y_{22} - Z_{22} \end{pmatrix}\begin{pmatrix} u^1 \\ \varphi^1 \end{pmatrix} + \begin{pmatrix} d_1^2 \\ d_2^2 \end{pmatrix}$, respectively.

We will continue with the presentation of numerical experiments regarding the *stability* of equation (3.1) (see Proposition 3.1). The shape of the graphs ploted in Figures 3 and 4 shows the stability and accuracy of the numerical results obtained by algorithm **Alg_1-IMBDF**. For this test we have used $T = 2$, $b = 1$, $M = 100$, $N = 40$ and the temperature surrounding at $\partial\Omega=\{0, b\}$ given by: $w(t_i, 0) = -15$, $w(t_i, b) = 7.5$, $i = 1, 2, ..., M$.

Taking now *k=.785*, we can verify that $v_{min} - v_{max}$=*-15.2372* which means that the first hypothesis in Proposition 3.1 in not verified. Consequently the numerical scheme is unstable. Figure 5 shows that it really is. Furthemore, if we keep *k=.785* and take τ=*1.0e+2**ξ^2 (in place of τ=*1.0e+3**ξ^2), we get also $v_{min} - v_{max} < 0$. So, again we are in a unstable case. Moreover, analyzing the graph in Figure 6 we found a more pronounced instability. Let's remark that the instability of the solution occurred following a slight change (modification) of only two physical parameters (k and τ in this case). This highlights the strong dependence of approximation scheme regarding physical parameters.

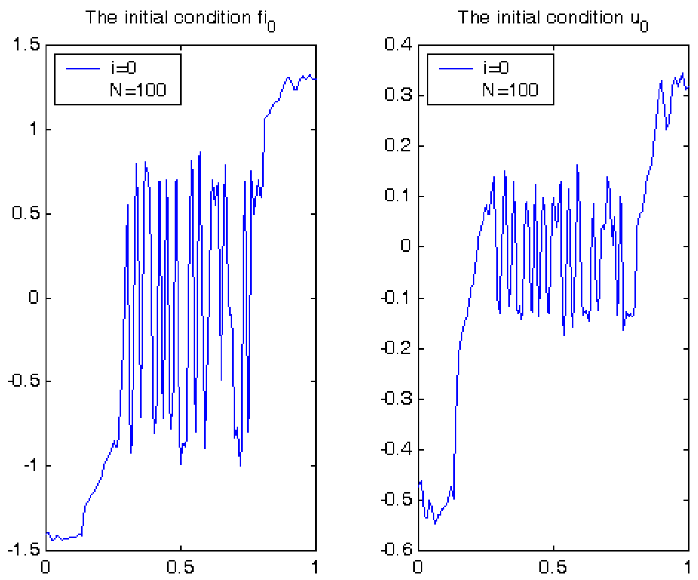

Fig. 1. The initial conditions φ_0 and u_0

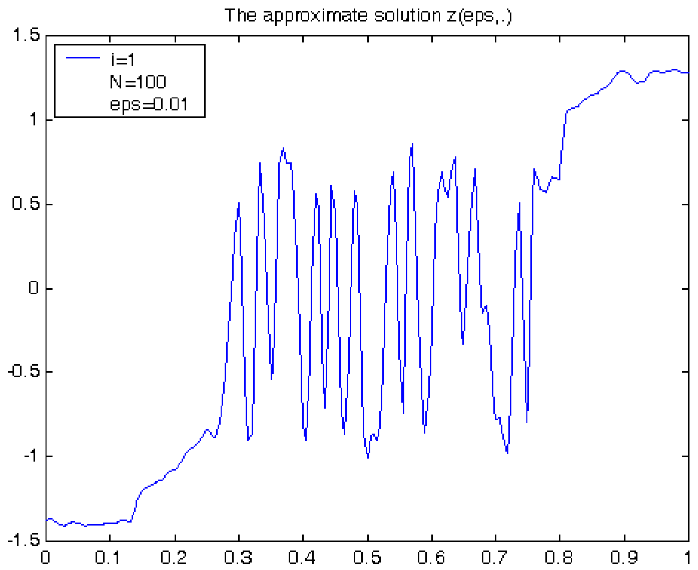

Fig. 2. The approximate solution $z(\varepsilon, \cdot)$ of Cauchy problem (1.7)

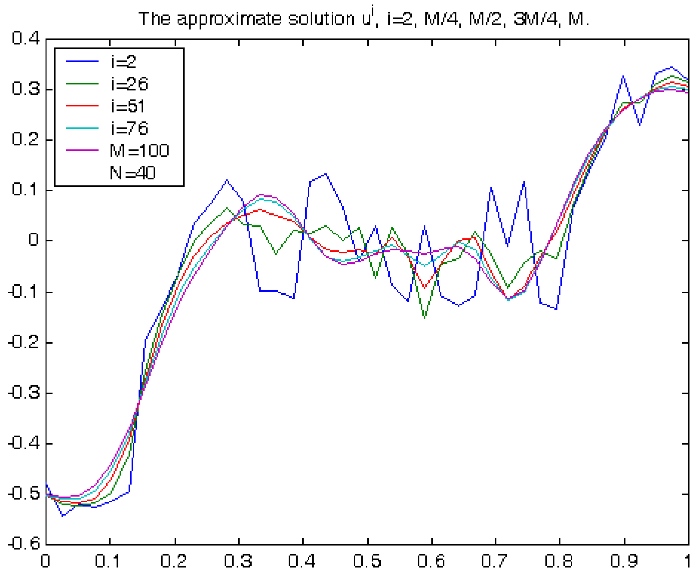

Fig. 3. Example of numerical stability: u^i at different levels of time

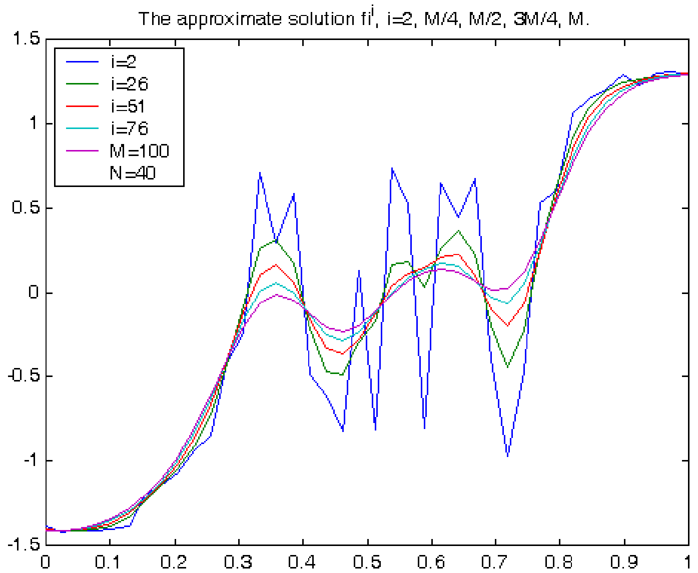

Fig. 4. Example of numerical stability: φ^i at different levels of time

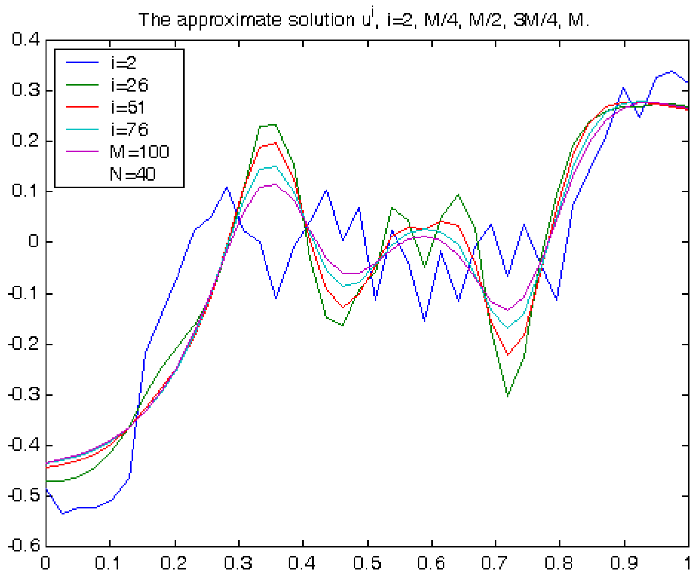

Fig. 5. An example of slight numerical instability

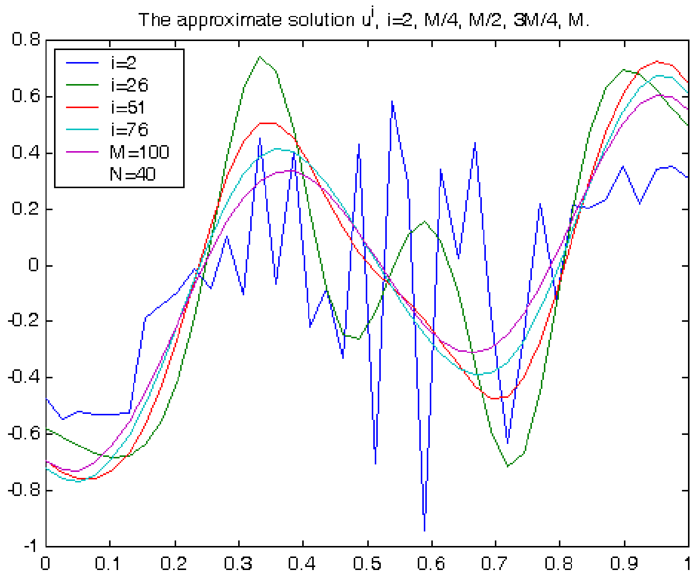

Fig. 6. An example of strong numerical instability

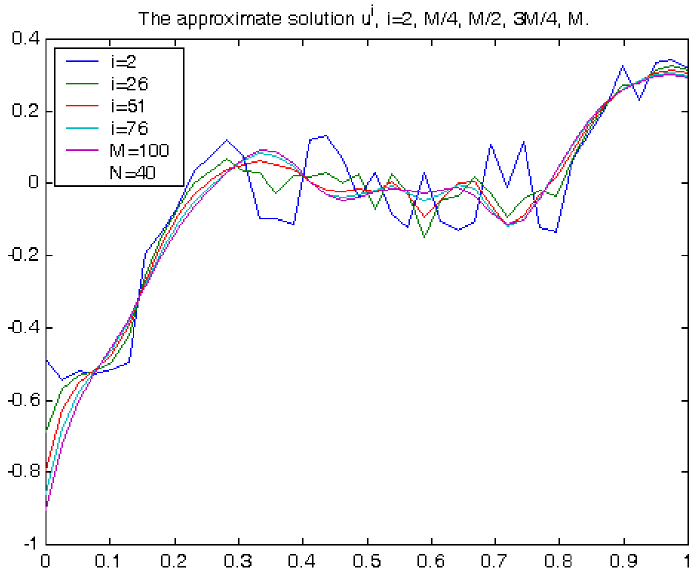

Fig. 7. u^i corresponding to $w^i(0) = -60$, via Alg_1-IMBDF

We turn to numerical stability conditions and we change the temperature surrounding at $0 \in \partial\Omega$ by setting $w(t_i, 0) = -60$, $i = 1, 2, ..., M$. The numerical results, obtained by algorithms **Alg_1-IMBDF** and **Alg_2-SBDF**, were ploted in Figures 7 and Figure 8 below, respectively. Analyzing the approximations near to zero, we observe a instability just for u, due to the nature of boundary conditions that we have considered $(1.2)_1$. In addition we also find a difference in the error of approximation.

On stability, we mention that similar results were also obtained by implementing the algorithms **Alg_2-IMBDF** and **Alg_2-SBDF**. In this sense, we reproduce in Figure 9 the numerical result obtained by Alg_2-IMBDF, executed with the same values as in Alg_1-IMBDF (see Figure3).

5. CONCLUSIONS

As the novelty of this work we notice the use of three finite difference schemes in order to approximate the linear system given by a scheme of fractional steps type. Even if each brings particularities in the implementation (memory space required, the right side), executed in the same conditions, produced essentially the same numerical results (see figures 3 and 9). Not least, let's remark that conditions of stability are sustained by both theory and numerical experiment and that are significantly dependent on the physical parameters.

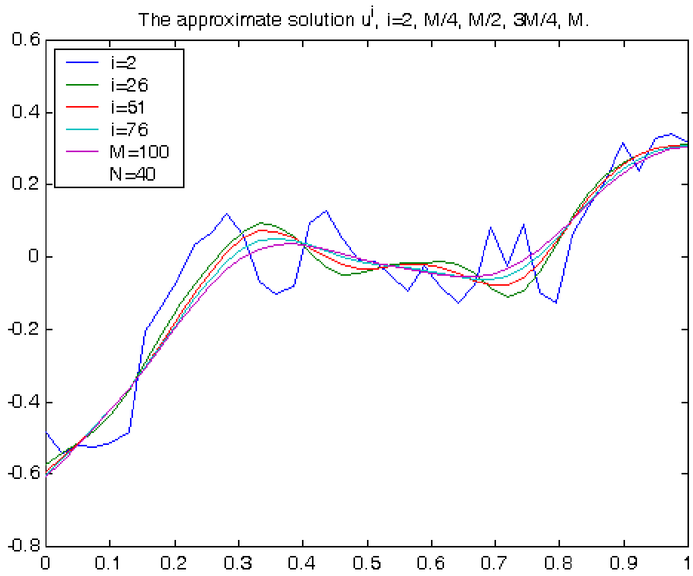

Fig. 8. u^i corresponding to $w^i(0) = -60$, via Alg_2-SBDF

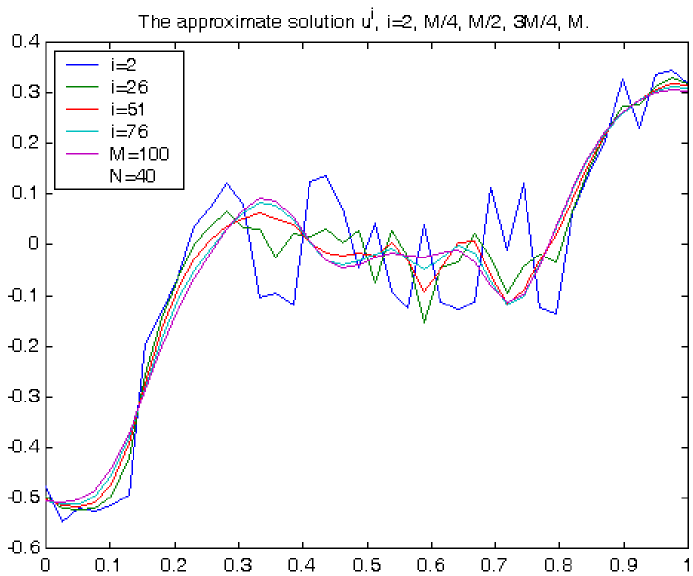

Fig. 9. u^i obtained by Alg_2-IMBDF

Analyzing the numerical results in terms of physical phenomena, we constat that *the temperature distribution* tends to become parabolic and *the phase function* distribution say that the instability of the portion of material will disappear. Moreover, analyzed together (see figures 3 and 4, for example), highlight theoretical meaning assigned to functions u and φ as well as the *zone of separation* between material phases.

The numerical solution obtained by this way can be considered as an admissible one for the corresponding boundary optimal control problem (from this perspective, compare figures 7 and 8). Generally, the numerical method considered here can be used to approximate the solution of a nonlinear parabolic phase-field system containing a general nonlinear part.

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