

**ON THE NUMERICAL
APPROXIMATION OF THE
NONLINEAR PHASE-FIELD
EQUATION SUPPLIED WITH
NON-HOMOGENEOUS DYNAMIC
BOUNDARY CONDITIONS. CASE 1D***

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Dedicated to the memory of Prof. Dr. Viorel Arnăutu

Abstract

The paper is concerned with the numerical analysis of a scheme of fractional steps type, associated to the nonlinear phase-field (Allen-Cahn) equation, endowed with non-homogeneous dynamic boundary conditions (depending both on the time and space variables). To approximate the solution of the linear parabolic equation, introduced by such approximating schemes, a first-order **IM**PLICIT **B**ACKWARD **D**IFFERENTIATION **F**ORMULA (**1-IMBDF**) is considered. A conceptual numerical algorithm and numerical experiments in one dimension are performed too.

MSC: 35K55, 65N06, 65N12, 65YXX, 80AXX

keywords: Boundary value problems for nonlinear parabolic PDE, fractional steps method, convergence of numerical method, computer aspects of numerical algorithm, phase-changes, dynamic boundary conditions.

*Accepted for publication in revised form on February 4-th, 2015

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1 Introduction

Consider the following nonlinear parabolic boundary value problem with respect to the unknown function φ :

$$\alpha\xi\frac{\partial}{\partial t}\varphi - \xi\Delta\varphi = \frac{1}{2\xi}(\varphi - \varphi^3) \quad \text{in } Q = [0, T] \times \Omega$$

$$\xi\frac{\partial}{\partial\nu}\varphi + \alpha\xi\frac{\partial}{\partial t}\varphi - \Delta_\Gamma\varphi + c_0\varphi = w(t, x) \quad \text{on } \Sigma = [0, T] \times \partial\Omega \quad (1.1)$$

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

where:

- Ω is a bounded domain in \mathbb{R}^n with boundary $\partial\Omega = \Gamma$ and $T > 0$ stands for some final time;
- $\varphi(t, x)$ is the *phase function* (used to distinguish between the states (phases) of a material which occupies the region Ω at every time $t \in [0, T]$);
- α (the *relaxation time*), ξ (the *measure of the interface thickness*) and c_0 are positive constants;
- Δ_Γ is the Laplace-Beltrami operator;
- $w(t, x) \in W_p^{1-\frac{1}{2p}, 2-\frac{1}{p}}(\Sigma)$ is a given function and p satisfies

$$p \geq \frac{3}{2}; \quad (1.2)$$
- $\varphi_0 \in W_\infty^{2-\frac{2}{p}}(\Omega)$ verifying $\xi\frac{\partial}{\partial\nu}\varphi_0 - \Delta_\Gamma\varphi_0 + c_0\varphi_0 = w(0, x)$ on Γ .

Equation (1.1)₁ was introduced initially by Allen and Cahn (see [1]) to describe the motion of anti-phase boundaries in crystalline solids. Actually, the Allen-Cahn model is widely applied to moving interface problems, such as the mixture of two incompressible fluids, the nucleation of solids, vesicle membranes, etc. Also, the nonlinear parabolic equation (1.1)₁ appears in the Caginalp's phase-field transition system (see [4]) describing the transition between the solid and liquid phases in the solidification process of a material occupying a region Ω (see [6]).

Following the strategy used in [5] and [9], the nonlinear parabolic boundary value problem (1.1) can be rewritten suitably in the following form:

$$\left\{ \alpha\xi \frac{\partial}{\partial t} \varphi - \xi \Delta \varphi = \frac{1}{2\xi} (\varphi - \varphi^3) \quad \text{in } Q, \varphi = \psi \right.$$

$$\text{on } \Sigma \xi \frac{\partial}{\partial \nu} \varphi + \alpha\xi \frac{\partial}{\partial t} \psi - \Delta_\Gamma \psi + c_0 \psi = w(t, x)$$

$$\text{on } \Sigma \varphi(0, x) = \varphi_0(x) \quad x \in \Omega, \psi(0, x) = \psi_0(x) \quad x \in \Gamma, \quad (1.3)$$

where the new variable $\psi = \varphi$, $\psi(0, x) = \varphi_0$ on Γ , is introduced in order to treat the dynamic boundary conditions (1.1)₂ as a parabolic equation for ψ on the boundary Γ , with $\psi_0 \in W_\infty^{2-\frac{2}{p}}(\Gamma)$, $\varphi_0 = \psi_0$ on Γ and, for the remaining data in (1.1), we keep the meanings already formulated.

As regards the existence in (1.3), it is known that under appropriate conditions on φ_0 and w , there exists a unique solution $(\varphi, \psi) \in W_p^{1,2}(Q) \times W_p^{1,2}(\Sigma)$, $p \geq \frac{3}{2}$ (see [5, Theorem 2.1]). Here we have used the standard notation for Sobolev spaces, namely, given a positive integer k and $1 \leq p \leq \infty$, we denote by $W_p^{k,2k}(Q)$ the usual Sobolev space on Q :

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

i.e., the space of functions whose t -derivatives and x -derivatives up to the order k and $2k$, respectively, belong to $L^p(Q)$. Also, we have used the Sobolev spaces $W_p^l(\Omega)$, $W_p^{\frac{l}{2},l}(\Sigma)$ with nonintegral l for the initial and boundary conditions, respectively (see [7, Chapter 1] and references therein).

Numerical investigation of the nonlinear parabolic problem (1.1), subject to various other types of boundary conditions, have been made in [2], [3], [7] and [8]. The main novelty of this work is the presence of the non-homogeneous dynamic boundary conditions (1.1)₂, untreated numerically until now (to our knowledge) in the mathematical literature and which makes the present nonlinear parabolic problem (1.1) to be more accurate in describing many important phenomena of two-phase systems: *superheating*, *supercooling*, *the effects of surface tension*, *separating zones*, etc; in particular, the interactions with the walls in confined systems. Consequently, a wide variety of industrial applications are covered.

In order to approximate the solution of the nonlinear boundary value problem (1.3) (in fact, the solution of problem (1.1)), a *scheme of fractional*

steps type was introduced and analyzed in [9], namely, for every $\varepsilon > 0$, it was associated to problem (1.3) the following approximating scheme (see also [2-3], [6-8]):

$$\begin{cases} \alpha\xi \frac{\partial}{\partial t} \varphi^\varepsilon - \xi \Delta \varphi^\varepsilon = \frac{1}{2\xi} \varphi^\varepsilon \text{ in } Q_i^\varepsilon \\ \xi \frac{\partial}{\partial \nu} \varphi^\varepsilon + \alpha\xi \frac{\partial}{\partial t} \psi^\varepsilon - \Delta_\Gamma \psi^\varepsilon + c_0 \psi^\varepsilon = w(t, x) \text{ on } \Sigma_i^\varepsilon \\ \varphi^\varepsilon(i\varepsilon, x) = z(\varepsilon, \varphi_-^\varepsilon(i\varepsilon, x)) \text{ on } \Omega, \psi^\varepsilon(i\varepsilon, x) = \varphi^\varepsilon(i\varepsilon, x) \text{ on } \Gamma, \end{cases} \quad (1.4)$$

where $Q_i^\varepsilon = [i\varepsilon, (i+1)\varepsilon] \times \Omega$, $\Sigma_i^\varepsilon = [i\varepsilon, (i+1)\varepsilon] \times \Gamma$ and $z(\varepsilon, \varphi_-^\varepsilon(i\varepsilon, x))$ is the solution of the Cauchy problem:

$$\begin{cases} z'(s) + \frac{1}{2\xi} z^3(s) = 0 & s \in [0, \varepsilon] \\ z(0) = \varphi_-^\varepsilon(i\varepsilon, x) & \text{on } \Omega \\ \varphi_-^\varepsilon(0, x) = \varphi_0(x) & \text{on } \Omega \\ \varphi_-^\varepsilon(0, x) = \psi_0(x) & \text{on } \Gamma, \end{cases} \quad (1.5)$$

for $i = 0, 1, \dots, M_\varepsilon - 1$, with $M_\varepsilon = \lceil \frac{T}{\varepsilon} \rceil$, $Q_{M_\varepsilon-1}^\varepsilon = [(M_\varepsilon - 1)\varepsilon, T] \times \Omega$, $\Sigma_{M_\varepsilon-1}^\varepsilon = [(M_\varepsilon - 1)\varepsilon, T] \times \Gamma$ and φ_-^ε stands for the left-hand limit of φ^ε .

In other words, the fractional steps method consists in decoupling the nonlinear problem (1.3) in a linear parabolic boundary value problem, expressed on a partition of the time interval $[0, T]$ (composed from M_ε subintervals, the first $M_\varepsilon - 1$ having the same length ε) and a nonlinear ordinary differential equation containing the nonlinearity φ^3 . Accordingly, the advantage of this approach consists in simplifying the numerical computation of the process of approximation for the solution of nonlinear problem (1.1).

Invoking again the Theorem 2.1 in [5], we have that there is a unique solution to (1.4)-(1.5), namely: $(\varphi^\varepsilon, \psi^\varepsilon) \in W_p^{1,2}(Q_i^\varepsilon) \times W_p^{1,2}(\Sigma_i^\varepsilon)$, with $p \geq \frac{3}{2}$ and $i = 0, 1, \dots, M_\varepsilon - 1$.

Owing to the Lions and Peetre embedding theorem, we know that $W_p^{1,2}(Q) \subset L^\infty(Q)$ if $p \geq \frac{3}{2}$ (see [7, Chapter 1] and references therein) and thus, for later use, we will introduce the sets:

$$W_Q = L^2([0, T]; H^1(\Omega)) \cap L^\infty(Q) \text{ and } W_\Sigma = L^2([0, T]; H^1(\Gamma)) \cap L^\infty(\Sigma).$$

Definition 1 *By a weak solution of the nonlinear problem (1.3) we mean a pair of functions $(\varphi, \psi) \in W_Q \times W_\Sigma$, $\varphi = \psi$ on Σ , which satisfies (1.3) in the following sense:*

$$\begin{aligned} & \alpha \xi \int_Q \left(\frac{\partial}{\partial t} \varphi, \phi_1 \right) dt dx + \xi \int_Q \nabla \varphi \nabla \phi_1 dt dx \\ & + \alpha \xi \int_\Sigma \left(\frac{\partial}{\partial t} \psi, \phi_2 \right) dt d\gamma + \int_\Sigma \nabla \psi \nabla \phi_2 dt d\gamma + c_0 \int_\Sigma \psi \phi_2 dt d\gamma \\ & = \frac{1}{2\xi} \int_Q (\varphi - \varphi^3) \phi_1 dt dx + \int_\Sigma w \phi_2 dt d\gamma \end{aligned} \quad (1.6)$$

$\forall (\phi_1, \phi_2) \in L^2([0, T]; H^1(\Omega)) \times L^2([0, T]; H^1(\Gamma))$, and $\varphi(0, x) = \varphi_0(x)$ in Ω .

The symbols \int_Q and \int_Σ above denote the duality between $L^2([0, T]; H^1(\Omega))$ and $L^2([0, T]; H^1(\Omega)')$, as well as $L^2([0, T]; H^1(\Gamma))$ and $L^2([0, T]; H^1(\Gamma)')$, respectively.

The following result (see [3], [7]) establishes the relationship between the solution (φ, ψ) in (1.3) and the solution $(\varphi^\varepsilon, \psi^\varepsilon)$ in (1.4)-(1.5).

Theorem 1 *Assume that $\varphi_0(x) \in W_\infty^{2-\frac{2}{q}}(\Omega)$, satisfying $\xi \frac{\partial}{\partial \nu} \varphi_0 - \Delta_\Gamma \varphi_0 + c_0 \varphi_0 = w(0, x)$ on Γ , and $w(t, x) \in W_p^{1-\frac{1}{2p}, 2-\frac{1}{p}}(\Sigma)$. Let $(\varphi^\varepsilon, \psi^\varepsilon)$ be the solution of the approximating scheme (1.4)-(1.5). Then for $\varepsilon \rightarrow 0$, one has*

$$(\varphi^\varepsilon, \psi^\varepsilon) \rightarrow (\varphi^*, \psi^*) \quad \text{strongly in } L^2(\Omega) \times L^2(\Gamma) \quad \text{for any } t \in (0, T], \quad (1.8)$$

where $(\varphi^*, \psi^*) \in W_Q \times W_\Sigma$ is the weak solution of the nonlinear equation (1.3).

The outline of the paper is as follows: in Section 2 we have introduced the discrete equations corresponding to (1.4)-(1.5); consequently, a conceptual numerical algorithm has been formulated: **Alg_1-IMBDF_dbc**. A stability result for this approach is stated and proved in the next Section. Some numerical experiments are reported in the last Section.

2 Numerical method

In this section we are concerned with the numerical approximation of the solution $(\varphi^\varepsilon, \psi^\varepsilon)$ to (1.4)-(1.5). As already stated, we will work in one

dimension and then $\Delta\varphi^\varepsilon = \varphi_{xx}^\varepsilon$, $\Delta_\Gamma\psi^\varepsilon = \psi_{xx}^\varepsilon$ and $\frac{\partial}{\partial\nu}\varphi^\varepsilon = \frac{\partial}{\partial x}\varphi^\varepsilon \cdot \nu = \mp\varphi_x^\varepsilon$ (i.e., (see [7, Chapter 1, p. 27]), the directional derivative of φ^ε in the direction of the outward pointing unit normal vector ν).

Let $\Omega = (0, b) \subset \mathbb{R}_+$ and we introduce over it the grid with N equidistant nodes

$$x_j = (j-1)dx \quad j = 1, 2, \dots, N, \quad dx = \frac{b}{N-1}.$$

Accordingly, the boundary Γ is given by the set of points $\{x_1=0, x_N=b\}$.

Considering $M \equiv M_\varepsilon$ as the number of equidistant nodes in which is divided the time interval $[0, T]$, we set

$$t_i = (i-1)\varepsilon \quad i = 1, 2, \dots, M, \quad \varepsilon = \frac{T}{M-1}.$$

We denote by φ_j^i the approximate values in the point (t_i, x_j) of the unknown function φ^ε . More precisely

$$\varphi_j^i = \varphi^\varepsilon(t_i, x_j) \quad i = 1, 2, \dots, M, \quad j = 1, 2, \dots, N,$$

i.e., for the later use

$$\varphi^i \stackrel{\text{not}}{=} (\varphi_1^i, \varphi_2^i, \dots, \varphi_N^i)^T \quad i = 1, 2, \dots, M. \quad (2.1)$$

We continue by explaining how we will treat each term from (1.4)-(1.5). Owing to the relation (1.4)₄ and knowing that $\Gamma = \{x_1, x_N\}$, we can put

$$\begin{aligned} \{\psi_1^i = \psi^\varepsilon(t_i, x_1) = \varphi^\varepsilon(t_i, x_1) = \varphi_1^i\psi_N^i = \psi^\varepsilon(t_i, x_N) = \varphi^\varepsilon(t_i, x_N) = \varphi_N^i \\ i = 1, 2, \dots, M. \end{aligned} \quad (2.2)$$

The Laplace operator in (1.4)₁ will be approximated by a *second order centered finite differences*, that is, for $i = 1, 2, \dots, M$:

$$\varphi_{xx}^\varepsilon(t_i, x_j) = \Delta_{dx}\varphi_j^i \approx \frac{\varphi_{j-1}^i - 2\varphi_j^i + \varphi_{j+1}^i}{dx^2} \quad j = 1, 2, \dots, N, \quad (2.3)$$

where Δ_{dx} is the discrete Laplace operator, depending on the step-size dx . Corresponding to the Laplace-Beltrami operator in (1.4)₂, we will use the same approximating scheme as above, which, correlated with (1.4)₄ and (2.2), gives us

$$\left\{ \begin{aligned} \psi_{xx}^\varepsilon(t_i, x_1) = \Delta_{dx}\psi_1^i \approx \frac{\varphi_0^i - 2\varphi_1^i + \varphi_2^i}{dx^2}\psi_{xx}^\varepsilon(t_i, x_N) = \Delta_{dx}\psi_N^i \end{aligned} \right.$$

$$\approx \frac{\varphi_{N-1}^i - 2\varphi_N^i + \varphi_{N+1}^i}{dx^2} \quad i = 1, 2, \dots, M, \quad (2.4)$$

where φ_0^i and φ_{N+1}^i are dummy variables.

Involving the separation of variables method to solve the Cauchy problem (1.5) (see [2], [6], [7], [8]), we obtain

$$\begin{cases} z(\varepsilon, \varphi_-^\varepsilon(t_1, x)) = z(\varepsilon, \varphi_0(x)) = \varphi_0(x) \sqrt{\frac{\xi}{\xi + \varepsilon \varphi_0(x)}}, z(\varepsilon, \varphi_-^\varepsilon(t_i, x)) = \\ \varphi_-^\varepsilon(t_i, x) \sqrt{\frac{\xi}{\xi + \varepsilon \varphi_-^\varepsilon(t_i, x)}} \quad i = 2, \dots, M - 1. \end{cases} \quad (2.5)$$

Remembering that $\partial\Omega = \Gamma = \{x_1, x_N\}$, the boundary conditions (1.4)₂ can be rewritten as follows

$$\left\{ -\xi \varphi_x^\varepsilon(x_1) + \alpha \xi \frac{\partial}{\partial t} \psi^\varepsilon(t_i, x_1) - \psi_{xx}^\varepsilon(t_i, x_1) + c_0 \psi^\varepsilon(t_i, x_1) = \right.$$

$$\left. w(t_i, x_1) \xi \varphi_x^\varepsilon(x_N) + \alpha \xi \frac{\partial}{\partial t} \psi^\varepsilon(t_i, x_N) - \psi_{xx}^\varepsilon(t_i, x_N) + c_0 \psi^\varepsilon(t_i, x_N) = w(t_i, x_N), \right. \quad (2.6)$$

for $i = 1, 2, \dots, M$, where the sign in the front of $\frac{\partial}{\partial \nu} \varphi^\varepsilon = \varphi_x^\varepsilon \cdot \nu$ is $-$ ($+$) because the normal to $[0 = x_1, b = x_N]$ at x_1 (x_N) point is in the negative (positive) direction (i.e. the unit normal vector $\nu = \mp 1$ at 0 and b , respectively).

Now, using in (2.6) a forward (backward) finite differences to approximate $\varphi_x^\varepsilon(x_1)$ ($\varphi_x^\varepsilon(x_N)$) and, taking into account the relations (2.2) and (2.4), we get

$$\left\{ -\xi \frac{\varphi_2^i - \varphi_1^i}{dx} + \alpha \xi \frac{\partial}{\partial t} \psi^\varepsilon(t_i, x_1) - \Delta_{dx} \psi_1^i + c_0 \psi_1^i = \right.$$

$$\left. w_1^i \xi \frac{\varphi_N^i - \varphi_{N-1}^i}{dx} + \alpha \xi \frac{\partial}{\partial t} \psi^\varepsilon(t_i, x_N) - \Delta_{dx} \psi_N^i + c_0 \psi_N^i = w_N^i, \right. \quad (2.7)$$

where $w_1^i = w(t_i, x_1)$, $w_N^i = w(t_i, x_N)$, $i = 1, 2, \dots, M$.

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

$$\begin{cases} \frac{\partial}{\partial t} \varphi^\varepsilon(t_i, x_j) \approx \frac{\varphi_j^i - \varphi_j^{i-1}}{\varepsilon} & i = 2, 3, \dots, M, \quad j = 1, 2, \dots, N \\ \frac{\partial}{\partial t} \psi^\varepsilon(t_i, x_j) \approx \frac{\psi_j^i - \psi_j^{i-1}}{\varepsilon} & i = 2, 3, \dots, M, \quad j \in \{1, N\}. \end{cases} \quad (2.8)$$

Finally we refer to the right hand in (1.4)₁ that is $\frac{1}{2\xi} \varphi^\varepsilon(t_i, x_j)$. To approximate this quantity (the *reaction term*), we will involve an implicit formula (see [8]), i.e.:

$$\frac{1}{2\xi} \varphi^\varepsilon(t_i, x_j) \approx \frac{1}{2\xi} \varphi_j^i \quad i = 1, 2, \dots, M, \quad j = 1, 2, \dots, N. \quad (2.9)$$

We are now ready to build the **1-IMBDF** approximating scheme. To do this, we begin by replacing in (1.4)₁ the approximations stated in (2.3), (2.8)₁ and (2.9). We deduce

$$\alpha\xi \frac{\varphi_j^i - \varphi_j^{i-1}}{\varepsilon} - \xi \Delta_{dx} \varphi_j^i = \frac{1}{2\xi} \varphi_j^i, \quad i = \overline{2, M}, \quad j = \overline{1, N}. \quad (2.10)$$

We continue by replacing in (1.4)₂ the approximations stated in (2.4), (2.7) and (2.8)₂ which leads to

$$\begin{cases} \alpha\xi \frac{\psi_1^i - \psi_1^{i-1}}{\varepsilon} - \xi \frac{\varphi_2^i - \varphi_1^i}{dx} - \Delta_{dx} \psi_1^i + c_0 \psi_1^i = w_1^i, \\ \alpha\xi \frac{\psi_N^i - \psi_N^{i-1}}{\varepsilon} + \xi \frac{\varphi_N^i - \varphi_{N-1}^i}{dx} - \Delta_{dx} \psi_N^i + c_0 \psi_N^i = w_N^i, \end{cases} \quad i = \overline{2, M}. \quad (2.11)$$

Substituting in (2.10) and (2.11) the approximations of $\Delta_{dx} \varphi_j^i$, $\Delta_{dx} \psi_1^i$ and $\Delta_{dx} \psi_N^i$, expressed by (2.3) and (2.4), respectively, using (2.2) and arranging convenient, we obtain that (1.4) is discretized as follows

$$\left\{ -c_2 \varphi_{j-1}^i + \left[c_1 + 2c_2 - \frac{1}{2\xi} \right] \varphi_j^i - c_2 \varphi_{j+1}^i = c_1 \varphi_j^{i-1} \quad j = \overline{1, N}, \right.$$

$$[c_1 + c_3 + 2 + c_0] \varphi_1^i - (1 + c_3) \varphi_2^i = w_1^i + c_1 \varphi_1^{i-1} + \varphi_0^i, \quad -(1 + c_3) \varphi_{N-1}^i +$$

$$[c_1 + c_3 + 2 + c_0] \varphi_N^i = w_N^i + c_1 \varphi_N^{i-1} + \varphi_{N+1}^i, \quad (2.12)$$

for $i = 2, 3, \dots, M$, where

$$c_1 = \frac{\alpha\xi}{\varepsilon}, \quad c_2 = \frac{\xi}{dx^2} \quad \text{and} \quad c_3 = \frac{\xi}{dx}.$$

In order to compute the matrix $(\varphi_j^i)_{i=2, \dots, M, j=1, \dots, N}$, the linear system (2.12) will be solved ascending with respect to the time levels. For the first time level ($i = 1$), the values of φ_j^1 are computed using (1.4)₃ and (2.5). For more details on implementing this computation process which involves the variable z , see the cycle "For $i = 2$ to M do" in the algorithm "Alg_1-IMBDF_dbc" listed below.

Moreover, let us point out from (2.12) that we have N unknowns for each time-level $i, i = 2, 3, \dots, M$ (see and (2.1)).

If, corresponding to $j = 1$ and $j = N$ we take $\varphi_0^i = \varphi_1^i$ and $\varphi_{N+1}^i = \varphi_N^i$, than the system (2.12) can be rewritten in matrix form as

$$A\varphi^i = B\varphi^{i-1} + d^i \quad i = 2, 3, \dots, M, \quad (2.13)$$

where

$$A = \begin{pmatrix} a_1 - (1 + c_2 + c_3)0 \cdots 000 - c_2c_1 + 2c_2 - \frac{1}{2\xi} - c_2 \cdots 000 \cdots \cdots \cdots 000 \cdots \\ -c_2c_1 + 2c_2 - \frac{1}{2\xi} - c_2000 \cdots 0 - (1 + c_2 + c_3)a_1 \end{pmatrix}$$

$$a_1 = c_1 + 2c_2 + c_3 + c_0 + 1 - \frac{1}{2\xi},$$

$$B = \begin{pmatrix} 2c_10 \cdots 000c_1 \cdots 00 \cdots \cdots \cdots 00 \cdots c_1000 \cdots 02c_1 & d^i = \begin{pmatrix} w_1^i 0 \cdots 0w_N^i \end{pmatrix} \end{pmatrix}$$

Therefore, the general design of the algorithm to calculate the approximate solution to the nonlinear system (1.4)-(1.5), via *fractional steps method* and *1-IMBDF*, is the following one

```

Begin Alg_1-IMBDF_dbc
  Choose  $T > 0, b > 0$ ;
  Choose  $M > 0, N > 0$ ; compute  $\varepsilon$  and  $dx$ ;
  Choose  $\varphi_0$  and  $w$ ;
  Set  $\psi_0(x_1) = \varphi_0(x_1)$  and  $\psi_0(x_N) = \varphi_0(x_N)$ ;
  Compute  $\varphi_1^1 = \varphi_-^\varepsilon(0, x_1) = \psi_0(x_1)$  from (1.5)4;
    
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For  $j = 2$  to  $N - 1$  do
  Compute  $\varphi_j^1 = \varphi_-^\varepsilon(0, x_j) = \varphi_0(x_j)$  from (1.5)3;
End-for;
Compute  $\varphi_N^1 = \varphi_-^\varepsilon(0, x_N) = \psi_0(x_N)$  from (1.5)4;
For  $i = 2$  to  $M$  do
  Compute  $w_1^{i-1}$  and  $w_N^{i-1}$ ;
  Compute  $\varphi^{i-1} = z(\varepsilon, \varphi_-^\varepsilon(t_{i-1}, \cdot))$  using (2.5);
  Compute  $\varphi^i$  solving the linear system (2.13);
End-for;
End.

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As it is well known, most initial value problems reduce to solving large sparse linear systems of the form (2.13). For later use regarding the numerical implementation of the conceptual algorithms **Alg_1-IMBDF_dbc**, we proof the following

Lemma 1. *If*

$$c_1 + 2c_2 + c_3 + c_0 + 1 - \frac{1}{2\xi} \neq 0 \quad \text{and} \quad c_1 + 2c_2 - \frac{1}{2\xi} \neq 0, \quad (2.14)$$

then the matrix coefficients in linear system (2.13) can be factored into the product of a lower-triangular matrix and an upper-triangular matrix (LU-factorization).

Proof. Let denote by a_{mn} , $m, n = 1, 2, \dots, N$, the elements of matrix coefficients in linear system (2.13). Analyzing the main diagonal elements of block matrices A , we first find that, owing to the hypothesis expressed by (2.14), second part, the coefficients a_{nn} , $n = 2, 3, \dots, N - 1 \neq 0$. Observing now that $a_1 \neq 0$ reflect the assumptions expressed in (2.14), first part, we find easily that $a_{nn} \neq 0 \forall n = 1, 2, \dots, N$. So Gaussian elimination can be performed on the system (2.13) without interchanges; consequently A has an LU factorization.

Remark 1. As we can easily deduce from the proof of Lemma 1, the hypothesis (2.14) expresses the requirement that all diagonal elements of the matrix coefficients A in (2.13) to be non-zero, which guarantees the existence of LU decomposition.

3 Stability conditions

To establish conditions of stability for the linear difference equations expressed by (2.13), we will use in our analysis the Lax-Richtmyer definition of

stability, expressed in terms of norm $\|\cdot\|_\infty$ (see [7, Chapter 5] and references therein). Equation (2.13) may be rewritten in a more convenient form as

$$\varphi^i = A^{-1}B\varphi^{i-1} + A^{-1}d^i \quad i = 2, 3, \dots, M \quad (3.1)$$

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

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

where $D = \text{diag}(a_1, c_1 + 2c_2 - \frac{1}{2\xi}, \dots, c_1 + 2c_2 - \frac{1}{2\xi}, a_1)$ and $G = A - D$. Thus, noting $a_2 = c_1 + 2c_2 - \frac{1}{2\xi}$, we have

$$D^{-1}G = \begin{pmatrix} 0 & \frac{1+c_2+c_3}{a_1} & 0 & \dots & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & \dots & 0 & 0 & \dots & 0 & 0 & \dots & 0 & 0 \\ -\frac{c_2}{a_2} & 0 & -\frac{c_2}{a_2} & \dots & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & \dots & 0 & 0 & \dots & 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \vdots & \vdots \\ 0 & \dots & 0 & \dots & 0 & \dots & 0 & \dots & 0 & \dots & 0 & \dots & 0 & \dots & 0 & \dots & 0 & \dots & 0 & \dots & 0 \end{pmatrix}$$

$$0 \quad \frac{1+c_2+c_3}{a_1} \quad 0$$

The sum of each line in matrix $D^{-1}G$ is written in the vector v below (recall that $a_1 = c_1 + 2c_2 + c_3 + c_0 + 1 - \frac{1}{2\xi}$ and $a_2 = c_1 + 2c_2 - \frac{1}{2\xi}$)

$$v = \left[-\frac{1+c_2+c_3}{a_1}, -2\frac{c_2}{a_2}, \dots, -2\frac{c_2}{a_2}, -\frac{1+c_2+c_3}{a_1} \right]. \quad (3.3)$$

Let's denote by

$$v_{max} = \max\{|-(1+c_2+c_3)|, |-2c_2|\} \quad \text{and} \quad v_{min} = \min\{|a_1|, |a_2|\}.$$

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

Proposition 1. *Suppose that $v_{min} - v_{max} > 0$. If*

$$\frac{\alpha\xi}{v_{min} - v_{max}} < \frac{\varepsilon}{2} \quad (3.4)$$

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

Proof. The proof is reduced to check the inequality $\|A^{-1}B\|_\infty < 1$. We begin by determining an estimate for $\|D^{-1}G\|_\infty = \max|v|$, wherefrom we easily derive the estimate

$$\|D^{-1}G\|_\infty < \frac{v_{max}}{v_{min}}. \quad (3.5)$$

The estimate (3.5) allows 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: $\|(I + D^{-1}G)^{-1}\|_\infty < \frac{1}{1 - \|D^{-1}G\|_\infty}$ and making use of (3.2), it follows that

$$\|A^{-1}\|_\infty \leq \|(I + D^{-1}G)^{-1}\|_\infty \|D^{-1}\|_\infty < \frac{1}{1 - \|D^{-1}G\|_\infty} \|D^{-1}\|_\infty. \quad (3.6)$$

How the inequality $\|D^{-1}G\|_\infty < 1$ imply that $1 - \|D^{-1}G\|_\infty > 1 - \frac{v_{max}}{v_{min}} > 0$, we easily deduce now that

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

Since $\|D^{-1}\|_\infty \leq \frac{1}{v_{min}}$ and involving the above estimate, from (3.6) we finally obtain

$$\|A^{-1}\|_\infty < \frac{1}{v_{min} - v_{max}}. \quad (3.7)$$

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

$$\|B\|_\infty = \max\{2c_1, c_1\} = 2\frac{\alpha\xi}{\varepsilon}. \quad (3.8)$$

Summing up and making use of (3.7)-(3.8) we derive the following estimate

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

which, owing to (3.4), leads us to the estimate $\|A^{-1}B\|_\infty < 1$ as we claimed at beginning of proof.

Remark 2. The hypothesis $v_{min} > v_{max}$ in Proposition 1 derives from the necessity to have a strict sub-unitary estimation for $\max|v|$ (see relation (3.3)). A large part of numerical experiments presented in the next section are designed to support this theoretical aspect.

4 Numerical experiments

The aim of this Section is to present numerical experiments implementing the conceptual algorithm **Alg 1-IMBDF_dbc**. Corresponding to input data T, b, M, N , we have used several different values, while, for the model's parameters, we have started with the values: $\xi = .5$, $\alpha = 1.0e + 1$ and $c_0 = 1.0e - 3$.

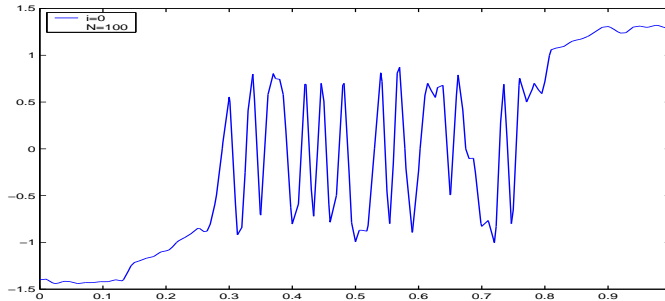


Figure 1: *The initial conditions φ_0*

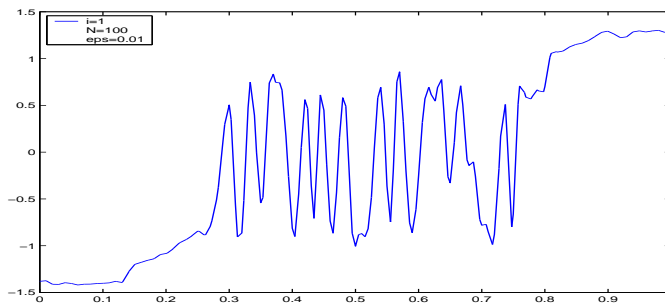


Figure 2: *The approximate solution $z(\varepsilon, \cdot)$ of the Cauchy problem (1.5)*

The initial values $\varphi_0(x_j)$, $j = 1, 2, \dots, N$, plotted in Figure 1, were computed via Matlab function `csapi(fi0)` - cubic spline interpolant, corresponding to the following input 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 -0.95 -0.9 -0.85 -0.88 -0.6 .0 .5 -0.92 -0.25 .8 -0.7 ...
      .58 .75 .58 -0.63 -0.59 .69 -0.72 .7 -0.59 -0.5 .7 -0.79 -0.87 -0.88 .0 .72 -0.8 .81 ...
      .0 -0.89 .0 .7 .55 .68 -0.49 .79 .0 -0.1 -0.8 -0.78 -0.83 .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];
```

Now (see (2.5)) we are able to calculate the vector $(z(\varepsilon, \varphi_0(x_j)))_{j=1, \overline{N}}$, plotted in Figure 2, and the vector $\varphi^1 = (\varphi_j^1)_{j=1, \overline{N}}$ (see (1.4)₃).

We will present now some numerical experiments regarding the *stability* of the matrix equation (3.1), established by Proposition 1. For the first tests, we have set: $T = 1$, $b = 2$, $M = 100$, $N = 100$ and the values at boundary given by: $w(t_i, 0) = -725$, $w(t_i, b) = 0$, $i = 1, 2, \dots, M$. We can verify that $v_{min} - v_{max} = 1.69e + 3 > 0$ and $\frac{\alpha\xi}{v_{min} - v_{max}} - \frac{\varepsilon}{2} = -0.0021 < 0$. Consequently, all hypothesis in Proposition 1 are satisfied and then we are

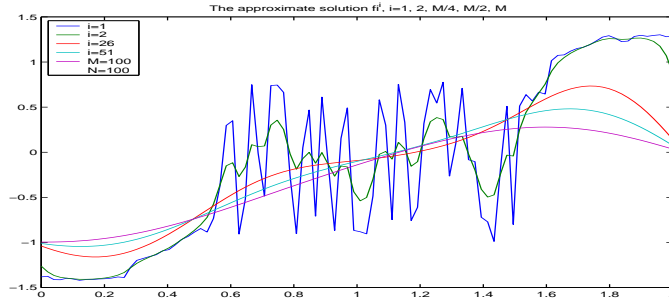


Figure 3: *Example of numerical stability: φ^i at different levels of time*

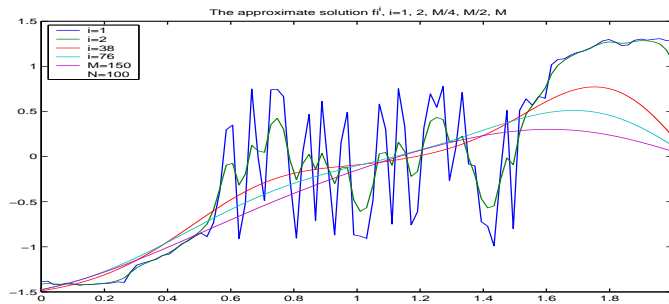


Figure 4: *Example of numerical stability: φ^i at different levels of time*

in a stability case. The shape of the graphs plotted in Figures 3 shows that it really is. Changing in the above settings only the value of M , again we are in a stable case. Analyzing the graph in Figure 4 we find a slight improvement of stability in the boundary point $x_1 = 0$.

Taking now $T = 2$, $b = 2$, $M = 50$, $N = 50$ and $\alpha = 1.0e + 2$, one can check that $\frac{\alpha\xi}{v_{min}-v_{max}} - \frac{\varepsilon}{2} = 0.00224 > 0$ which means that the hypothesis (3.4) is not verified, i.e., the numerical scheme (3.1) is unstable (see Figure 5). Changing $\xi = 0.75$ and $c_0 = 1.0e + 3$, we get $\frac{\alpha\xi}{v_{min}-v_{max}} - \frac{\varepsilon}{2} = 0.0054 > 0$. So, again we are in a unstable case (see Figure 6). Let's remark that the instability of the solution occurred after a slight change for α , ξ and c_0 . This highlights the strong dependence of approximation scheme regarding physical parameters.

We turn to numerical stability conditions changing $w(t_i, 0) = 72.5$ and $w(t_i, b) = -72.5$, $i = 1, 2, \dots, M$. We get again a stable case and the numerical results, obtained by algorithms **Alg_1-IMBDF dbc** were plotted in Figure 7. Analyzing the approximations near 0 and b , we observe a good stability which makes it suitable to be used in the numerical analysis of the

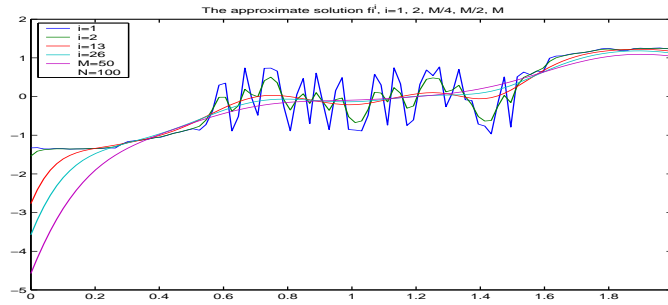


Figure 5: *Example of a numerical instability*

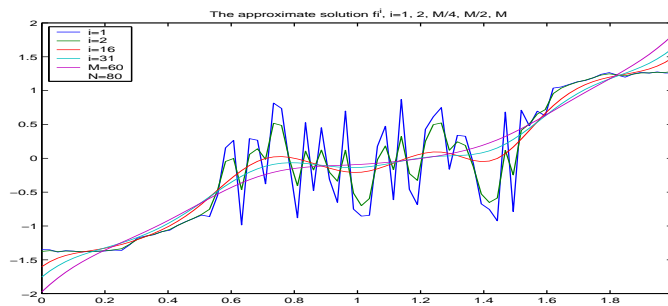


Figure 6: *Example of a slight numerical instability*

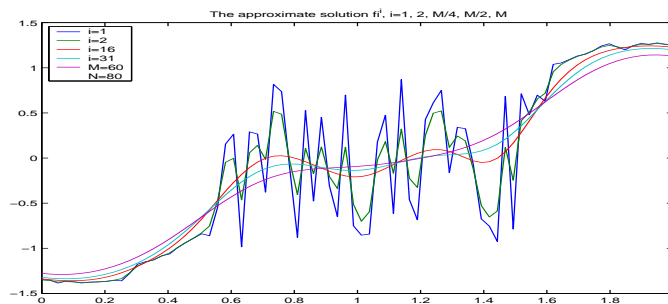


Figure 7: *Example of numerical stability: φ^i at different levels of time*

boundary optimal control problems governed by (1.1).

5 Conclusions

Analyzing the numerical results in terms of physical phenomena (see figures 3-7), we find that *the phase function* distribution say that the instability of the portion of material will disappear. Moreover, the numerical experiments depicted in figure 7, for example, highlight the theoretical meaning assigned to the unknown function φ and the *zone of separation* between material phases.

The numerical solution obtained by this way can be considered as an admissible one for the appropriate boundary optimal control problem (from this perspective, compare figures 4, 5 and 7 in terms of stability). 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. Not the 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.

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