

ON THE NUMERICAL APPROXIMATION OF A NONLINEAR REACTION-DIFFUSION EQUATION WITH NON-HOMOGENEOUS NEUMANN BOUNDARY CONDITIONS. CASE 1D

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Abstract The paper concerns with an implicit first-order in time, finite- differences in space, method to solve numerically a reaction-diffusion equation endowed with a cubic nonlinearity, and non-homogeneous Neumann boundary conditions. Numerical tests for the Allen-Cahn equation are presented and analyzed in terms of the physical quantities of interest.

Keywords: nonlinear PDE of parabolic type; finite difference methods, Newton method; fractional steps method; thermodynamics, phase changes.

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1. INTRODUCTION

We consider the following nonlinear and nonlocal reaction-diffusion equation for the unknown function $v(t, x)$

$$p_1 \frac{\partial}{\partial t} v(t, x) = p_2 \left\{ \int_{\Omega} J(x-y) [v(t, y) - v(t, x)] dy + \int_{\partial\Omega} J(x-y) w(t, y) d\gamma \right\} \\ + p_3 [v(t, x) - v^3(t, x)] + \frac{p_3}{|\Omega|} \int_{\Omega} [v(t, y) - v^3(t, y)] dy \quad (1)$$

in $Q = (0, T] \times \Omega$, with initial condition

$$v(0, x) = v_0(x), \quad (2)$$

where:

- $T > 0$ stands for some final time and Ω is a bounded domain in \mathbb{R}^n , whose boundary $\partial\Omega$ is smooth enough. Of course, $t \in (0, T]$, while x and y varies in Ω ;
- $v(t, x)$ is the unknown function: a real-valued order parameter. In particular, $v(t, x)$ is the *phase function* (used to distinguish between the states (phases) of a material which occupies the region Ω at every time $t \in (0, T]$);
- $\frac{\partial}{\partial t}v(t, x)$ is the partial derivative of $v(t, x)$ with respect to t ;
- $J : \mathbb{R} \rightarrow \mathbb{R}$ is symmetric continuous nonnegative real function, compactly supported in the unit ball, and such that $\int_{\mathbb{R}} J(z)dz = 1$;
- p_1, p_2, p_3 are positive values. p_2 measures the strength of interactions at sites x and y ;
- $w(t, x) \in L_{loc}^\infty((0, \infty), L^1(\Gamma))$;
- $v_0(x) \in L^1(\Omega)$ stands for the initial condition.

More details on certain interpretations of the terms $J(x - y)$, $\int_{\Omega} J(x-y)v(t, y)dy$, $-\int_{\Omega} J(x-y)v(t, x)dy$ and $\frac{1}{|\Omega|} \int_{\Omega} f(v(t, y))dy$ in the mathematical model (1), can be found in the works P. W. Bates, S. Brown and J. Han [11], P. C. Fife [22], S. Pavăl [28], O. Penrose and P. C. Fife [29], J. Rubinstein and P. Sternberg [30], I. Stoleriu [33], and references therein.

The nonlocal reaction-diffusion equation (1)-(2) can be seen as similar to the local reaction-diffusion equation with non-homogeneous Neumann boundary conditions (see M. Bogoya and J. Gómez [13], C. Cortazar, M. Elgueta, J.D. Rossi and N. Wolanski [19]), namely:

$$\left\{ \begin{array}{ll} p_1 \frac{\partial}{\partial t} v(t, x) = p_2 \Delta v(t, x) + p_3 [v(t, x) - v^3(t, x)] + \frac{p_3}{|\Omega|} \int_{\Omega} [v(t, y) - v^3(t, y)] dy & \text{in } Q, \\ p_2 \frac{\partial}{\partial \mathbf{n}} v(t, x) = w(t, x) & \text{in } \Sigma, \\ v(0, x) = v_0(x) & \text{on } \Omega, \end{array} \right. \quad (3)$$

where $\Sigma = (0, T] \times \Gamma$ and $\mathbf{n}=\mathbf{n}(\mathbf{x})$ is a vector of the outward (from Ω) unit normal to the surface Σ . $\frac{\partial}{\partial \mathbf{n}}$ denotes differentiation along \mathbf{n} .

The nonlinear problems (1)-(2) and (3) are important for modeling a variety of phenomena of life sciences (material science, in particular).

The behaviour of solutions to the nonlocal model (1)-(2) when one rescales the kernel J considering $J(z) = \frac{1}{\varepsilon^3} J(\frac{z}{\varepsilon})$ are studied in M. Bogoya and J. Gómez [13] while for the numerical solutions we refer to P. W. Bates, S. Brown and J. Han [11] and I. Stoleriu [33].

Problem (3) is a particular instance of the Allen-Cahn equation [1], which was introduced to describe the motion of anti-phase boundaries in crystalline solids, and it has been widely applied to many complex moving interface problems, e.g., the *mixture of two incompressible fluids*, the *nucleation of solids*, the *vesicle membranes* (see for instance P. W. Bates, S. Brown and J. Han [11], M. Bogoya and J. Gómez [13], X. Chen [18], P. de Mottoni and M. Schatzman [20], X. Feng and A. Prohl [21], P. C. Fife [22], H. G. Lee and J.-Y. Lee [19], J. Shen and X. Yang [32], X. Yang [34], J. Zhang and Q. Du [35] and the references therein). Also, the nonlinear problems (3)₁, occurs in the phase-field transition system (see G. Caginalp and P. C. Fife [14], for example) where the phase function $v(t, x)$ describes the transition between the solid and liquid phases in the solidification process of a material occupying a region Ω . For more general assumptions and with various types of boundary conditions, equation (3) has been numerically investigated in e.g., V. Arnăutu and C. Moroşanu [10], T. Benincasa and C. Moroşanu [12], G. Caginalp and J.-T. Lin [15], C. I. Gheorghiu and C. Moroşanu [15], W. Hundsdorfer and J. Verwer [16], G. Iorga, C. Moroşanu and I. Tofan [18], A. de Masi, E. Orlandi, E. Presutti and L. Triolo [20], C. Moroşanu [21]-[24], C. Moroşanu and A.-M. Moşneagu [25], C. Moroşanu, S. Pavăl and C. Trenchea [26], A. A. Ovono [27], and I. Stoleriu [33]. The error analysis for the implicit backward Euler approximation is presented in C. Moroşanu, S. Pavăl and C. Trenchea [26]. Computations with several different higher-order time-stepping schemes are used in C. Moroşanu and A.-M. Moşneagu [25], J. Shen [31] while for the existence, estimate, uniqueness and regularity of a solution in Sobolev spaces we refer to O. Cârjă, A. Miranville, and C. Moroşanu [16], J. G. Carr, R. L. Pego [17], L. I. Ignat and J. D. Rossi [17] and C. Moroşanu [21].

1.1. APPROXIMATING SCHEME

The aim of this Subsection is to use the *fractional steps method* in order to approximate the solution of the nonlinear problem (1). To do that, let us associate to the time-interval $[0, T]$ the equidistant grid of length $\varepsilon_M = \frac{T}{M}$, for any integer $M \geq 1$, and corresponding to it, the approximate problem (4)-(6)

written below ($i = 0, 1, \dots, M - 1$):

$$\left\{ \begin{array}{l} p_1 \frac{\partial}{\partial t} v_M(t, \cdot) = p_2 \left\{ \int_{\Omega} J(x-y) [v_M(t, y) - v_M(t, x)] dy + \right. \\ \qquad \qquad \qquad \left. + \int_{\partial\Omega} J(x-y) w(t, y) d\gamma \right\} + \\ \qquad \qquad \qquad + \frac{p_3}{|\Omega|} \int_{\Omega} [v_M(t, y) - v_M^3(t, y)] dy \end{array} \right. \quad (4)$$

in $[i\varepsilon_M, (i+1)\varepsilon_M]$, with the initial condition

$$v_M(i\varepsilon_M, \cdot) = z_M(\varepsilon_M, \cdot), \quad (5)$$

where $z_M(\varepsilon_M, \cdot)$ is the solution of Cauchy problem

$$\left\{ \begin{array}{l} z'_M(\tau, \cdot) + p_3 [z_M(\tau, \cdot) - z_M^3(\tau, \cdot)] = 0, \quad \tau \in [0, \varepsilon_M], \\ z_M(0, \cdot) = v_M^-(i\varepsilon_M, \cdot), \quad v_M^-(0, \cdot) = v_0(x) \end{array} \right. \quad (6)$$

while v_M^- stands for the left-hand limit of v_M at $i\varepsilon_M$, that is: $v_M^-(i\varepsilon_M, \cdot) = \lim_{t \uparrow i\varepsilon_M} v_M(t, \cdot)$.

We point out that the sequence of approximating problems (4)-(6) supplies a decoupling method for the original problem (1)-(2) into a linear parabolic boundary value problem (4)-(5) and a nonlinear evolution equation (6). The advantage of this approach consists in simplifying the numerical computation of the approximations to (1)-(2), due to that the fractional steps method avoids the iterative process in passing from a time level to the next one.

Remark. *In the sequel, we will assume that for all $v_0 \in W_\infty^{2-\frac{2}{p}}(\Omega) \subset L^p(\Omega)$, $p \geq 2$, the sequence $\{v_M\}$ solving (4)-(6) converges to the unique solution v of problem (1)-(2), uniformly with respect to $[0, T]$ (see [10], [12], [21]-[23], [27] for a detailed discussion).*

The rest of the paper is organized as follows: in Section 2 we have introduced the discrete equation corresponding to (1), (3) and (4)-(6); consequently, conceptual algorithms: `Nonloc-Newton1D`, `Local-Newton1D` and `Nonloc-FracStep1D`, have been formulated. Some numerical experiments, implementing the above algorithms, are reported in Section 3 and some concluding remarks are presented in the last Section.

2. NUMERICAL METHODS

In this Section we are concerned with the numerical approximation of the solution $v(t, x)$ in (1), (3) and $v_M(t, x)$ in (4)-(6).

To fix the ideas, let $\Omega = [0, c] \subset \mathbb{R}_+$ and we introduce over it the grid with N equidistant nodes

$$x_j = (j - 1)h \quad j = 1, 2, \dots, N, \quad h = c/(N - 1).$$

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

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

Let's denote by v_j^i the approximate values in the point (t_i, x_j) of the unknown function $v(t, x)$ in (1) and (3), i.e.

$$v_j^i = v(t_i, x_j) \quad i = 1, 2, \dots, M, \quad j = 1, 2, \dots, N,$$

or, for later use

$$v^i = (v_1^i, v_2^i, \dots, v_N^i)^T \quad i = 1, 2, \dots, M. \quad (7)$$

From the initial condition (2) and (3)₃, we have

$$v_j^1 = v(t_1, x_j) = v_0(x_j) \quad j = 1, 2, \dots, N. \quad (8)$$

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

$$\frac{\partial}{\partial t} v(t_i, x_j) \approx \frac{v_j^i - v_j^{i-1}}{\varepsilon} \quad i = 2, \dots, M, \quad j = 1, 2, \dots, N. \quad (9)$$

To approximate the nonlinear term (*reaction term*) $[v(t, x) - v^3(t, x)]$ in (1) and (3)₁, we will involve an implicit formula, i.e.:

$$[v(t_i, x_j) - v^3(t_i, x_j)] \approx [v_j^i - (v_j^i)^3] \quad i = 1, 2, \dots, M, \quad j = 1, 2, \dots, N. \quad (10)$$

2.1. ALGORITHM NONLOC-NEWTON1D.

We will continue by approximating the terms remaining in (1). The *diffusion term* will be approximated by

$$\begin{aligned} & \int_{\Omega} J(x - y) [v(t, y) - v(t, x)] dy + \int_{\partial\Omega} J(x - y) w(t, y) d\gamma \approx \\ & \approx \left[(J * v^i)_j - v_j^i (J * 1)_j + (J * w^i)_j \right], \end{aligned} \quad (11)$$

with

$$(J * v^i)_j = h \left[\frac{1}{2} J(x_1 - x_j) v_1^i + \sum_{n=2}^{N-1} J(x_n - x_j) v_n^i + \frac{1}{2} J(x_N - x_j) v_N^i \right],$$

$$(J * 1)_j = h \left[\frac{1}{2} J(x_1 - x_j) + \sum_{n=2}^{N-1} J(x_n - x_j) + \frac{1}{2} J(x_N - x_j) \right],$$

$$(J * w^i)_j = \frac{1}{2} [J(x_1 - x_j)w_1^i + J(x_N - x_j)w_N^i],$$

where $w_1^i = w(t_i, 0)$, $w_N^i = w(t_i, c)$, $i = 1, 2, \dots, M$.

Finally, the *mass conserving term* will be approximated by

$$\int_{\Omega} [v(t, y) - v^3(t, y)] dy \approx \sum_{j=1}^N \frac{v_j^i - (v_j^i)^3}{h}. \quad (12)$$

We are now ready to build the approximation scheme, as we have mentioned at beginning. We begin by replaying in (1) the approximations stated in (9)-(12); we get:

$$\begin{aligned} & \frac{p_1}{\varepsilon} v_j^{i+1} - p_3 v_j^{i+1} + p_3 (v_j^{i+1})^3 \\ &= \frac{p_1}{\varepsilon} v_j^i + p_2 \left[(J * v^i)_j - v_j^i (J * 1)_j + (J * w^i)_j \right] + \frac{p_3}{|\Omega|} \sum_{j=1}^N \frac{v_j^i - (v_j^i)^3}{h}, \end{aligned} \quad (13)$$

for $i = 1, 2, \dots, M - 1$, $j = 1, 2, \dots, N$.

Arranging suitable and setting $c_1 = p_1 - \varepsilon p_3$, the discrete system (13) can be written in matrix form as follows

$$A v^i + \varepsilon p_3 \text{diag} \left((v_j^i)^3 \right)_{j=1, \dots, N} = p_1 v^{i-1} + d^i \quad i = 2, 3, \dots, M, \quad (14)$$

where

$$A = \begin{pmatrix} c_1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & c_1 & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & c_1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & c_1 \end{pmatrix}_{N \times N}$$

and

$$d^i = \varepsilon (d_1^i, d_2^i, \dots, d_N^i)^T,$$

with

$$d_1^i = p_2 \left[(J * v^i)_1 - v_1^i (J * 1)_j + (J * w^i)_1 \right] + \frac{p_3}{|\Omega|} \sum_{j=1}^N \frac{v_j^i - (v_j^i)^3}{h},$$

$$d_j^i = p_2 \left[(J * v^i)_j - v_j^i (J * 1)_j \right] + \frac{p_3}{|\Omega|} \sum_{j=1}^N \frac{v_j^i - (v_j^i)^3}{h} \quad j = 2, 3, \dots, N-1,$$

$$d_N^i = p_2 \left[(J * v^i)_N - v_N^i (J * 1)_N + (J * w^i)_N \right] + \frac{p_3}{|\Omega|} \sum_{j=1}^N \frac{v_j^i - (v_j^i)^3}{h}.$$

We shall now present the usual iterative Newton method in order to approximate the vector-solution v^i in (14) for time level i (we omit the upper index i - see (7)), i.e.

$$v = (v_1, v_2, \dots, v_N)^T.$$

From (14) it follows that we have to solve a nonlinear equation of the form $Y(v) = 0$. We recall that the iterative Newton method was

$$v^{(k+1)} = v^{(k)} - [Y'(v^{(k)})]_{N \times N}^{-1} Y(v^{(k)}), \quad (15)$$

where k is the iteration index. In our situation (14), we have

$$Y(v) = Av^i + \varepsilon p_3 \text{diag} \left((v_j^i)^3 \right)_{j=1, \overline{N}} - p_1 v^{i-1} - d^i,$$

$$Y'(v) = B + 3c_3 \text{diag} \left((v_j^i)^2 \right)_{j=1, \overline{N}},$$

with $Y = (Y_1, Y_2, \dots, Y_{N-1}, Y_N)^T$ given by

$$Y_j(v) = c_1 v_j^i + \varepsilon p_3 (v_j^i)^3 - p_1 v_j^{i-1} - \varepsilon d_j^i \quad j = 1, 2, \dots, N.$$

Thus, $v^{(k+1)}$ from (15) is the solution v of the linear system

$$[Y'(v^{(k)})]v = [Y'(v^{(k)})]v^{(k)} - Y(v^{(k)}). \quad (16)$$

The numerical algorithm to calculate the approximate solution in (1)-(2) by Newton method is the following one (i denotes the time level)

Begin Nonloc-Newton1D

$i := 1 \rightarrow v^1$ from the initial conditions (8);

For $i := 2$ to M do

 Establish the nonlinear system (14) to pass from $i-1$ to i ;

 Repeat (k)

 Newton iteration (16)

 Until convergence;

End-for;

End.

2.2. ALGORITHM LOCAL-NEWTON1D.

Let's come back to the nonlinear problem (3).

The Laplace operator $\Delta v(t, x) = v_{xx}(t, x)$ in (3)₁ (the *diffusion term*), will be approximated by a second order centred finite differences, namely:

$$v_{xx}(t_i, x_j) = \Delta_h v_j^i \approx \frac{v_{j-1}^i - 2v_j^i + v_{j+1}^i}{h^2} \quad i = 1, 2, \dots, M, \quad j = 1, 2, \dots, N, \quad (17)$$

(Δ_h is the discrete Laplacian depending on the step-size h).

Corresponding to Ω , already choosen in one dimension, the boundary $\partial\Omega$ is reduced to the set $\{0, c\}$. Thus the boundary conditions (3)₂ become

$$-p_2 v_x(0) = w(t, 0) \quad p_2 v_x(c) = w(t, c), \quad (18)$$

where the sign in front of $\frac{\partial}{\partial\nu} v = v_x$ is \mp because the normal to $[0, c]$ at 0 (c) point in the negative (positive) direction.

Using in (18) a forward (backward) finite differences to approximate $v_x(0)$ ($v_x(c)$), we get

$$-p_2 \frac{v_2^i - v_1^i}{h} = w^i(0) \quad p_2 \frac{v_N^i - v_{N-1}^i}{h} = w^i(c) \quad i = 1, 2, \dots, M, \quad (19)$$

i.e.

$$-p_2 [v_2^i - v_1^i] = h w_1^i \quad p_2 [v_N^i - v_{N-1}^i] = h w_N^i \quad i = 1, 2, \dots, M. \quad (20)$$

Next, by replaying in (3) the approximations stated in (9), (10), (12) and (17), we get:

$$\begin{aligned} p_1 v_j^{i+1} + \varepsilon p_2 \left[\frac{v_{j-1}^{i+1} - 2v_j^{i+1} + v_{j+1}^{i+1}}{h^2} \right] + \varepsilon p_3 \left[\left(v_j^{i+1} \right)^3 - v_j^{i+1} \right] &= p_1 v_j^i + \\ &+ \frac{\varepsilon p_3}{|\Omega|} \sum_{j=1}^N \frac{v_j^i - (v_j^i)^3}{h}, \end{aligned} \quad (21)$$

for $i = 1, 2, \dots, M - 1, j = 1, 2, \dots, N$.

Arranging suitable, making use of (20) and setting

$$c_1 = -\varepsilon \frac{p_2}{p_1} \frac{1}{h^2}, \quad c_2 = 1 - 2c_1 - \varepsilon \frac{p_3}{p_1}, \quad c_3 = \varepsilon \frac{p_3}{p_1},$$

than the discrete system (21) can be written in matrix form as follows

$$B v^i + c_3 \operatorname{diag} \left((v_j^i)^3 \right)_{j=1, \dots, N} = p_1 v^{i-1} + d^i, \quad (22)$$

where

$$B = \begin{pmatrix} c_1 + c_2 + p_2 & c_1 + p_2 & 0 & \cdots & 0 & 0 & 0 \\ c_1 & c_2 & c_1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & c_1 & c_2 & c_1 \\ 0 & 0 & 0 & \cdots & 0 & c_1 - p_2 & c_1 + c_2 + p_2 \end{pmatrix}_{N \times N}$$

and

$$d^i = \varepsilon (d_1^i, d_2^i, \dots, d_{N-1}^i, d_N^i)^T,$$

with

$$\begin{aligned} d_1^i &= \frac{p_3}{|\Omega|} \sum_{j=1}^N \frac{v_j^i - (v_j^i)^3}{h} + h w_1^i, \\ d_j^i &= \frac{p_3}{|\Omega|} \sum_{j=1}^N \frac{v_j^i - (v_j^i)^3}{h} \quad j = 2, 3, \dots, N-1, \\ d_N^i &= \frac{p_3}{|\Omega|} \sum_{j=1}^N \frac{v_j^i - (v_j^i)^3}{h} + h w_N^i. \end{aligned}$$

$i = 2, 3, \dots, M$.

In order to approximate the vector-solution v^i in (22) for time level i , $i = 2, 3, \dots, M$ (see (7), (8)), the usual iterative Newton method was involved too (see [15] for more details). In our new situation (22) (see and (15) in Subsection 2.1 with Z in place of Y), we have

$$\begin{aligned} Z(v) &= Bv^i + c_3 \text{diag} \left((v_j^i)^3 \right)_{j=1, \overline{N}} - p_1 v^{i-1} - d^i, \\ Z'(v) &= B + 3c_3 \text{diag} \left((v_j^i)^2 \right)_{j=1, \overline{N}}, \end{aligned}$$

with $Z = (Z_1, Z_2, \dots, Z_{N-1}, Z_N)^T$ given by

$$\begin{aligned} Z_1(v) &= (c_1 + c_2 + p_2)v_1^i + (c_1 + p_2)v_2^i + c_3(v_1^i)^3 - p_1 v_1^{i-1} - \varepsilon d_1^i, \\ Z_j(v) &= c_1 v_j^i + c_3(v_j^i)^3 - p_1 v_j^{i-1} - \varepsilon d_j^i \quad j = 2, \dots, N-1, \\ Z_N(v) &= (c_1 - p_2)v_{N-1}^i + (c_1 + c_2 + p_2)v_N^i + c_3(v_N^i)^3 - p_1 v_N^{i-1} - \varepsilon d_N^i, \end{aligned}$$

$i = 2, 3, \dots, M$.

Thus, $v^{(k+1)}$ (see (15)) is the solution v of the linear system

$$[Z'(v^{(k)})]v = [Z'(v^{(k)})]v^{(k)} - Z(v^{(k)}). \tag{23}$$

The numerical algorithm to calculate the approximate solution in (3) by Newton method is the following one (i denotes the time level)

Begin Local-Newton1D

$i := 1 \rightarrow v^1$ from the initial conditions (8);

For $i := 2$ to M do

Establish the nonlinear system (22) to pass from $i-1$ to i ;

Repeat (k)

Newton iteration (23)

Until convergence;

End-for;

End.

2.3. ALGORITHM NONLOC-FRACSTEP1D.

In this Subsection we are concerned with the numerical approximation of the solution $v_M(t, x)$ in (4)-(6). To fix the ideas, let the grid with N equidistant nodes: $x_j = (j-1)h$, $j = 1, 2, \dots, N$, $h = c/(N-1)$, associated to the space $\Omega = [0, c] \subset \mathbb{R}_+$, as well as the grid with M equidistant nodes: $t_i = i\varepsilon_M$, $i = 0, 1, 2, \dots, M-1$, $\varepsilon_M = T/M$, in which is divided the time interval $[0, T]$.

To solve the Cauchy problem (6), we will rewrite (6)₁ in an equivalent form, that is

$$u'(\tau, \cdot) = -2p_3 u(\tau, \cdot) + 2p_3 \quad \tau \in [0, \varepsilon_M], \quad (24)$$

where $u(\tau, \cdot) = z_M^{-2}(\tau, \cdot)$.

The solution of the linear equation (24) is given by

$$u(\varepsilon_M) = z_M(0, \cdot) \exp^{-2p_3 \varepsilon_M} + 2p_3 \varepsilon_M$$

and thus the solution of the Cauchy problem (6) is given by

$$z_M(\varepsilon_M, \cdot) = \frac{z_M(0, \cdot)}{\sqrt{z_M^3(0, \cdot) \exp^{-2p_3 \varepsilon_M} + 2p_3 \varepsilon_M z_M^2(0, \cdot)}}. \quad (25)$$

Let's denote by V_j^i the approximate values in the point $(i\varepsilon_M, x_j)$, ($i = 0, 1, 2, \dots, M-1$, $j = 1, 2, \dots, N$) of the unknown function $v_M(t, x)$ in (4), $(t, x) \in [0, T] \times [0, c]$, i.e.

$$V_j^i = v_M(i\varepsilon_M, x_j) \quad i = 1, 2, \dots, M, \quad j = 1, 2, \dots, N,$$

or, for later use

$$V^i = (V_1^i, V_2^i, \dots, V_N^i)^T \quad i = 1, 2, \dots, M. \quad (26)$$

From the initial condition (6)₂, we have

$$V^0 = v_0(x_j) \quad j = 1, 2, \dots, N. \quad (27)$$

Next, we introduce the discrete state equation corresponding to the approximate problem (4)-(6) as follows :

$$\left\{ \begin{array}{l} p_1 \frac{V^i - \phi^{i-1}}{\varepsilon_M} = p_2 \left[(J * V^{i-1})_j - V_j^{i-1} (J * 1)_j + (J * w^i)_j \right] + \\ \quad + \frac{p_3}{|\Omega|} \sum_{j=1}^N \frac{V_j^{i-1} - (V_j^{i-1})^3}{h} \\ \phi^{i-1} = v_M(i\varepsilon_M, \cdot), \end{array} \right. \quad (28)$$

$i = 1, 2, \dots, M$.

Therefore, the general design of the algorithm to compute the approximate solution of nonlinear system (1)-(2), via *fractional steps method* (4)-(6), is the following one

Begin Nonloc-FracStep1D

Choose $T > 0$, $c > 0$;
 Choose $M > 0$, $N > 0$ and compute ε_M, h ;
 Choose v_0, w ;
 $i := 0 \rightarrow V^0$ from the initial conditions (27);
 $v_M^-(0, \cdot) = V^0$;
 For $i = 1$ to M do
 $z_M(0, \cdot) = v_M^-((i-1)\varepsilon_M, \cdot)$;
 Compute $z_M(\varepsilon_M, \cdot)$ using (25);
 $v_M(i\varepsilon_M, \cdot) = z_M(\varepsilon_M, \cdot)$ (see (5)) ;
 $\Phi^{i-1} = v_M(i\varepsilon_M, \cdot)$;
 Compute V^i solving the explicit scheme (28);
 $v_M^-((i-1)\varepsilon_M, \cdot) = V^i$;
 End-for;
 End.

3. NUMERICAL EXPERIMENTS

This section presents numerical tests implementing the conceptual algorithms **Nonloc-Newton1D**, **Local-Newton1D** and **Nonloc-FracStep1D** (see previous section). Regarding the proposed difference scheme (13), we rescale the kernel J considering $J(x) = \frac{1}{\varepsilon} J\left(\frac{x}{\varepsilon}\right)$.

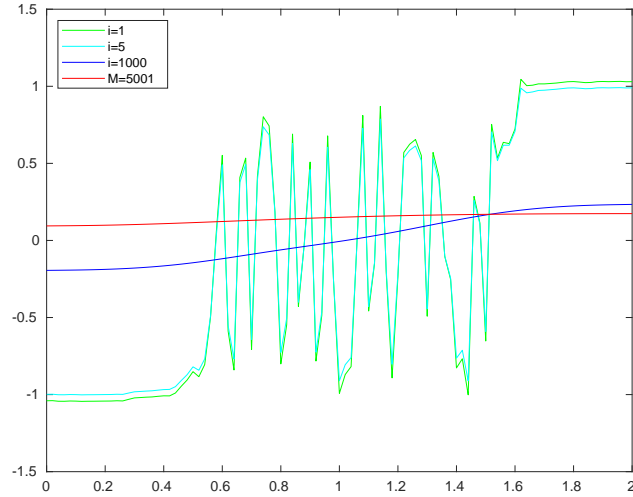


Fig. 1. The approximate solutions v^i at different levels of time: **Nonlocal-Newton1D**

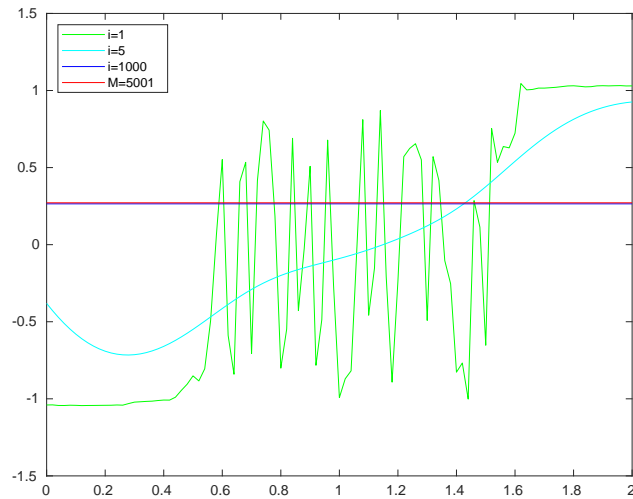


Fig. 2. The approximate solutions v^i at different levels of time: **Local-Newton1D**

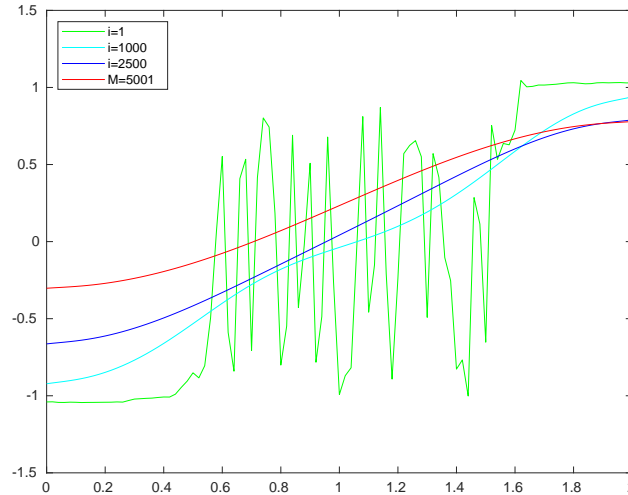


Fig. 3. The approximate solutions V^i at different levels of time: **Nonlocal_FracStep1D**

The initial values $v_0(x_j)$, $j = 1, 2, \dots, N$ (see (8) and (27)), were computed via Matlab function `csapi(v0)` - cubic spline interpolant to the given data (see Figures 3-6 for $i = 1$):

```
v0=[-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 -0.8 .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 numerical tests consider the Allen-Cahn equation, i.e., in the nonlinear reaction-diffusion equation (1) and (3) we take $p_1 = \alpha * \xi$, $p_2 = \xi$, $p_3 = \frac{1}{2\xi}$, when for the rescaled kernel we consider $J\left(\frac{x}{\varepsilon}\right) = \exp\left(-\left(\frac{x}{\varepsilon}\right)^2\right)$ (see [11]).

For beginning, taking $T = 5$, $c = 2$, $M = 5001$, $N = 101$, $\alpha = 1.0$, $\xi = .5$, the Figure 3-2 shows the numerical results at $t = 0.005$, $t = 1$, $t = 2.5$ and $t = 5$, corresponding to $w = 0$.

Next, we consider $\alpha = 0.1$, $\xi = 10\sqrt{5}$, $w_1^i = 0.006$ and $w_N^i = -0.005$, $i = 1, 2, \dots, M$. The approximate solutions v^i (V^i) at different time levels ($i = 5, 1000, 2500, 5001$) are plotted in Figures 3-6.

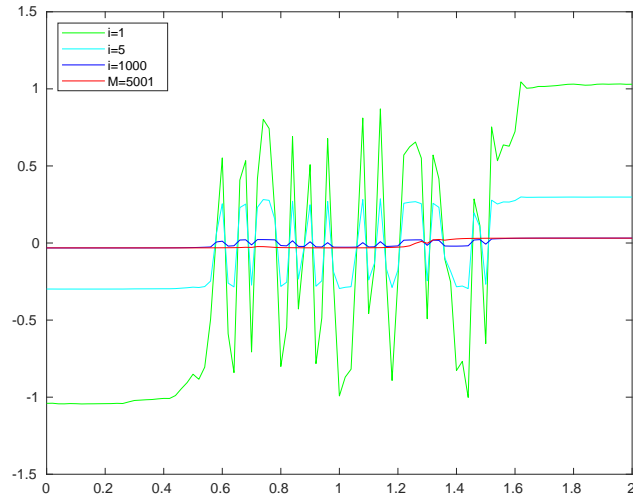


Fig. 4. The approximate solutions v^i at different levels of time: Nonlocal Newton1D

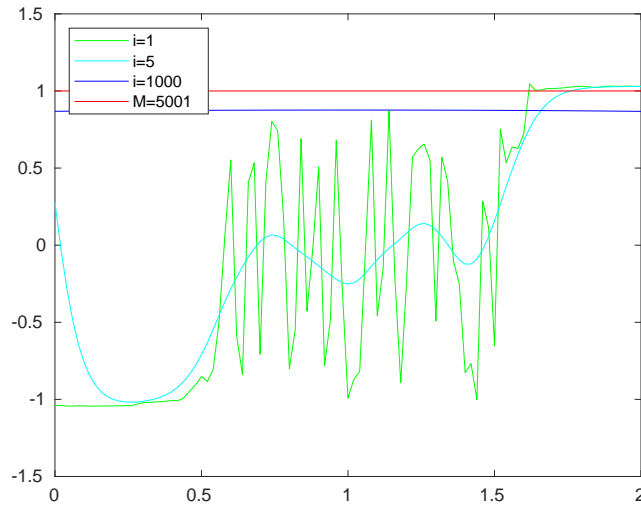


Fig. 5. The approximate solutions v^i at different levels of time: Local Newton1D

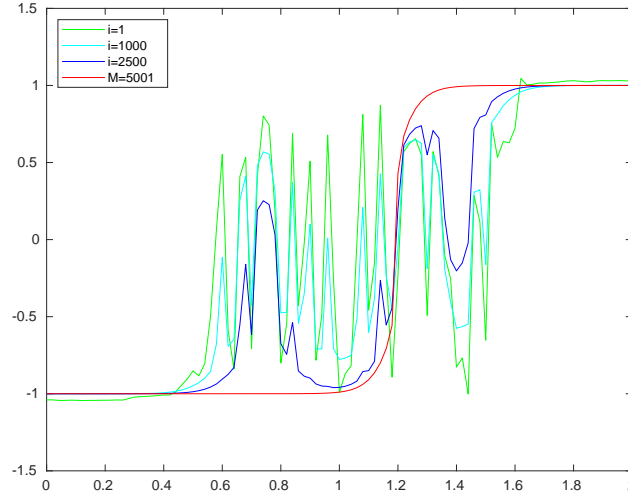


Fig. 6. The approximate solutions V^i at different levels of time: **Nonlocal_FracStep1D**

4. CONCLUSIONS

As a novelty of this work we refer to the numerical scheme introduced by (13), (21) and (28) in order to approximate the solution to the nonlocal reaction-diffusion problem (1) and (3) in presence of the cubic nonlinearity $v(t, x) - v^3(t, x)$, $(t, x) \in (0, T] \times [0, c]$ and the *mass conserving term*

$$\frac{p_3}{|\Omega|} \int_{\Omega} [v(t, y) - v^3(t, y)] dy.$$

Corresponding, we have considered an IMEX scheme and in the numerical experiments we focus our attention on a particular case of (1), (3) - the Allen-Cahn equation, which serves as a mathematical model for many complex moving interface problems and in which the challenge in terms of numerical analysis is due to the thickness of the interface separating different phases.

Next, let's remark that the numerical experiment, produced by the Newton method (16) and (23), are significantly influenced by the boundary input $w(t, x)$ (see [15], [25] and [26] for more details). Precisely, analyzing the graphical representation of the approximate solutions in terms of physical phenomena (the *phases* of the material occupying the region Ω at the time $t \in (0, T]$, for example), we constat that the instability disappeared from the whole region (see Figures 3-4 for the time level $i = 5001$). To the best of our knowledge, the present work presents for the first time results on the numerical solutions

for a nonlocal reaction-diffusion problem stated by (1), (3) and (4)-(6). New numerical methods as well as various numerical applications, are topics that we intend to deal with in the future. Not least, let's point out (as another open problem) that the approximate solutions obtained by implementing the numerical algorithms **Nonloc-Newton1D**, **Local-Newton1D** and **Nonloc-FracStep1D** can be regarded as admissible for the corresponding boundary optimal control problem.

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