NUMERICAL APPROXIMATION FOR A NONLOCAL REACTION-DIFFUSION EQUATION SUPPLIED WITH NON-HOMOGENEOUS NEUMANN BOUNDARY CONDITIONS. CASE 1D

Silviu Pavăl
Faculty of Automatic Control and Computer Engineering, “Gheorghe Asachi” Technical University, Iași, Romania
silviu.paval@tuiasi.ro

Abstract
The paper concerns with a first-order implicit difference scheme to solve numerically a nonlocal reaction-diffusion equation subject to the non-homogeneous Neumann boundary conditions. Numerical experiments are presented and analyzed in terms of physical phenomena, for a particular case of nonlocal reaction-diffusion equation: the Allen-Cahn equation.

Keywords: reaction-diffusion equations; finite difference methods, thermodynamics, phase changes.

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1. INTRODUCTION

Consider the following problem

\[
\begin{aligned}
\frac{p_1}{p_2} v_t(t,x) &= \\
&= \left\{ \int_{\Omega} J(x-y)[v(t,y)-v(t,x)] \, dy + \int_{\partial \Omega} J(x-y)w(t,y) \, d\gamma \right\} \\
&\quad + p_3 f(v(t,x)) + \frac{1}{|\Omega|} \int_{\Omega} f(v(t,y)) \, dy \\
&\quad \text{in } Q = (0,T] \times \Omega \\
v(0,x) &= v_0(x) \quad \text{on } \Omega,
\end{aligned}
\]

(1)

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 $\Omega$.

- $v(t, x)$ 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 $\Omega$ at every time $t \in (0, T]$);

- $f(v(t, x)) = F'(v(t, x))$ and $F(v(t, x)) = \frac{1}{4} (v^2(t, x) - 1)^2$. We assume that $f$ is smooth, $f(\pm 1) = 0 < f'(\pm 1)$ and has exactly one other zero that lies in $(-1, 1)$, i.e. $f$ is of bistable type;

- $v_t$ is the partial derivative of $v(t, x)$ with respect to $t$;

- $J : \mathbb{R} \to \mathbb{R}$ is symmetric continuous nonnegative real function, compactly supported in the unit ball, and such that $\int_{\mathbb{R}} J(z) \, dz = 1$;

- $p_2 > 0$ measures the strength of interactions at sites $x$ and $y$;

- $p_1, p_3$ are positive values;

- $w(t, x) \in L^\infty_{loc}((0, \infty), L^1(\Gamma))$;

- $v_0(x) \in L^1(\Omega)$ 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 by readers in the works of P. W. Bates, S. Brown and J. Han [3], P. C. Fife [14], O. Penrose and P. C. Fife [28], J. Rubinstein and P. Sternberg [29], I. Stoleriu [32] as well as the references therein.

The nonlocal reaction-diffusion equation (1) can be seen as similar to the local reaction-diffusion equation with non-homogeneous Neumann boundary conditions (see M. Bogoya and J. Gómez [5], C. Cortazar, M. Elgueta, J.D. Rossi and N. Wolanski [11])

\[
\begin{align*}
\begin{cases}
   p_1 v_t(t, x) &= p_2 \Delta v(t, x) + p_3 f(v(t, x)) + \frac{1}{|\Omega|} \int_{\Omega} f(v(t, y)) \, dy & \text{in } Q \\
   p_2 \partial_n v(t, x) &= w(t, x) & \text{in } \Sigma = (0, T] \times \Gamma \\
   v(0, x) &= v_0(x) & \text{on } \Omega,
\end{cases}
\end{align*}
\]

(2)
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where:

- \( \mathbf{n} = \mathbf{n}(x) \) is a vector of the outward (from \( \Omega \)) unit normal to the surface \( \Sigma \); \( \frac{\partial}{\partial \mathbf{n}} \) denotes differentiation along \( \mathbf{n} \).

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

The behavior of solutions to the nonlocal model (1) when one rescales the kernel \( J \) considering \( J(z) = \frac{1}{\varepsilon^3} J(\varepsilon z) \) are studied in M. Bogoya and J. Gómez [5] while for the numerical solutions we refer to P. W. Bates, S. Brown and J. Han [3] and I. Stoleriu [32].

Problem (2) it 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 [3], M. Bogoya and J. Gómez [5], X. Chen [10], P. de Mottoni and M. Schatzman [12], X. Feng and A. Prohl [9], P. C. Fife [14], H. G. Lee and J.-Y. Lee [19], J. Shen and X. Yang [31], X. Yang [34], J. Zhang and Q. Du [35] and the references therein). Also, the nonlinear problems (2) occurs in the phase-field transition system (see G. Caginalp and P. C. Fife [6], 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 \( \Omega \). For more general assumptions and with various types of boundary conditions, equation (2) has been numerically investigated in e.g., V. Arnăutu and C. Moroşanu [2], T. Benincasa and C. Moroşanu [4], G. Caginalp and J.-T. Lin [7], 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 [32]. 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 [30] while for the existence, estimate, uniqueness and regularity of a solution in Sobolev spaces we refer to O. Cârjă, A. Miranville, and C. Moroşanu [8], J. G. Carr, R. L. Pego [9], L. I. Ignat and J. D. Rossi [17], C. Moroşanu [21] and R. Temam [33].

The rest of the paper is organized as follows: in Section 2 we have introduced the discrete equation corresponding to (1); consequently, a conceptual algorithm have been formulated. Some numerical experiments are reported in Section 3 and the concluding remarks are formulated in the last Section.
2. NUMERICAL METHOD

In this Section we are concerned with the numerical approximation of the solution \( v(t, x) \) in (1). To fix the ideas, let \( \Omega = [0, c] \subset \mathbb{R}_+ \) and we introduce over it the grid with \( N \) equidistant nodes

\[
x_j = (j - 1)h \quad j = 1, 2, \ldots, N, \quad h = c/(N - 1).
\]

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

\[
t_i = (i - 1)\varepsilon \quad i = 1, 2, \ldots, M, \quad \varepsilon = T/(M - 1).
\]

Let’s denote by \( v^i_j \) the approximate values in the point \((t_i, x_j)\) of the unknown function \( v(t, x) \) in (1), i.e.

\[
v^i_j = v(t_i, x_j) \quad i = 1, 2, \ldots, M, \quad j = 1, 2, \ldots, N,
\]

or, for later use

\[
v^i = (v^i_1, v^i_2, \ldots, v^i_N)^T \quad i = 1, 2, \ldots, M. \tag{3}
\]

From the initial condition (1), we have

\[
v^1_j = v(t_1, x_j) = v_0(x_j) \quad j = 1, 2, \ldots, N. \tag{4}
\]

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

\[
v_i(t_{i+1}, x_j) \approx \frac{v^i_{j+1} - v^i_j}{\varepsilon} \quad i = 1, 2, \ldots, M - 1, \quad j = 1, 2, \ldots, N. \tag{5}
\]

To approximate the nonlinear term (reaction term) \( f(v(t, x)) = v(t, x) - v^3(t, x) \) in (1), we will involve an implicit formula, i.e.:

\[
[v(t_i, x_j) - v^3(t_i, x_j)] \approx [v^i_j - (v^i_j)^3] \quad i = 1, 2, \ldots, M, \quad j = 1, 2, \ldots, N. \tag{6}
\]

The diffusion term will be approximated by

\[
\int_{\Omega} J(x-y) \left[ v(t, y) - v(t, x) \right] dy + \int_{\partial\Omega} J(x-y)w(t, y) d\gamma \approx \left[ (J * v^i)_j - v^i_j (J * 1)_j + (J * w^i)_j \right],
\]

with

\[
(J * v^i)_j = \frac{1}{2} J(x_1 - x_j) v^i_1 + \sum_{n=2}^{N-1} J(x_n - x_j) v^i_n + \frac{1}{2} J(x_N - x_j) v^i_N,
\]

\[\int_{\partial\Omega} J(x-y)w(t, y) d\gamma \approx \left[ (J * w^i)_j \right] \]
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\[ (J * 1)_j = h \left[ \frac{1}{2} J(x_1 - x_j) + \sum_{n=2}^{N-1} J(x_n - x_j) + \frac{1}{2} J(x_N - x_j) \right], \]

and

\[ (J * w^i)_j = \frac{1}{2} [J(x_1 - x_j)w^i_1 + J(x_N - x_j)w^i_N], \]

where \( w^i_1 = w(t, 0), w^i_N = w(t_i, c), i = 1, 2, ..., M. \)

Finally, the mass conserving term will be approximated by

\[ \frac{1}{|\Omega|} \int_{\Omega} [v(t, y) - v^3(t, y)] dy \approx \frac{1}{|\Omega|} \sum_{j=1}^{N} \frac{v^i_j - (v^i_j)^3}{h}. \]  

First-order Implicit Backward Difference Formula (1-IMBDF). 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 (5)-(8); we get:

\[ \frac{p_1}{\varepsilon} v^{i+1}_j - p_3 v^{i+1}_j + p_3 \left( v^{i+1}_j \right)^3 = \frac{p_1}{\varepsilon} v^i_j + p_2 \left[ (J * v^i)_j - v^i_j (J * 1)_j + (J * w^i)_j \right] + \frac{1}{|\Omega|} \sum_{j=1}^{N} \frac{v^i_j - (v^i_j)^3}{h}, \]

for \( i = 1, 2, \ldots, M - 1, j = 1, 2, \ldots, N. \)

Arranging suitable and setting \( c_1 = p_1 - \varepsilon p_3, \) than the discrete system (9) can be written in matrix form as follows

\[ Av^i + \varepsilon p_3 \text{diag} \left( \left( v^i_j \right)^3 \right)_{j=1}^{N} = p_1 v^{i-1} + d^i \quad i = 2, 3, \ldots, M, \]  

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

\[ d^i = \varepsilon \left( d^i_1, d^i_2, \ldots, d^i_N \right)^T, \]

with

\[ d^i_1 = p_2 \left[ (J * v^i)_1 - v^i_1 (J * 1)_j + (J * w^j)_1 \right] + \frac{1}{|\Omega|} \sum_{j=1}^{N} \frac{v^i_j - (v^i_j)^3}{h}. \]
Algorithm Nonloc-Newton1D. We shall now present the usual iterative Newton method in order to approximate the vector-solution \( v^i \) in (10) for time level \( i \) (we omit the upper index \( i \)), i.e.

\[
v = (v_1, v_2, \cdots, v_N)^T.
\]

From (10) it follows that we have to solve a nonlinear equation of the form \( Y(v) = 0 \). We recall that the iterative Newton method was

\[
v^{(k+1)} = v^{(k)} - \left[ Y'(v^{(k)}) \right]^{-1} Y(v^{(k)}),
\]

where \( k \) is the iteration index. In our situation (10), (11) we have

\[
Y(v) = Av^i + \varepsilon p_3 \text{diag} \begin{pmatrix} (v_j^i)^3 \end{pmatrix}_{j=1}^{N} - p_1 v^{i-1} + d^i,
\]

\[
Y'(v) = A + 3 \varepsilon p_3 \text{diag} \begin{pmatrix} (v_j^i)^2 \end{pmatrix}_{j=1}^{N},
\]

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

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

Thus, \( v^{(k+1)} \) from (11) is the solution \( v \) of the linear system

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

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

Begin Nonloc-Newton1D

\[
i := 1 \rightarrow v^1 \quad \text{from the initial conditions (4)};
\]

For \( i := 2 \) to \( M \) do

Establish the nonlinear system (10) to pass from \( i-1 \) to \( i \);

Repeat \((k)\)

Newton iteration (12)

Until convergence;

End-for;

End.
3. NUMERICAL EXPERIMENTS

The aim of this section is to present some numerical experiments implementing the conceptual algorithm Nonloc-Newton1D in order to show that the proposed difference scheme (9) gives reasonable solutions.

We rescale the kernel $J$ considering $J(x) = \frac{1}{\varepsilon} J\left(\frac{x}{\varepsilon}\right)$ and for the initial conditions we will take the function $v_0(x) = \cos 2\pi x$ (see Figures 1-4 for $i = 1$).

![The approximate solution, via Newton: l=1, 2, 5, M.](image)

*Fig. 1.* The approximate solutions $v^i$ at different levels of time and $w = 0$

In the numerical tests we will consider a particular case of the nonlinear reaction-diffusion equation (1), namely, the Allen-Cahn equation ([1]), which means $p_1 = \alpha \ast \xi$, $p_2 = \xi$, $p_3 = \frac{1}{2\pi}$, when for the rescaled kernel we consider $J\left(\frac{x}{\varepsilon}\right) = \exp\left(-\left(\frac{x}{\varepsilon}\right)^2\right)$ (see [3]).

For beginning, taking $T = 0.1$, $c = 2$, $M = 101$, $N = 201$, $\alpha = 1.0$, $\xi = .5$, the Figure 1 shows the numerical results at $t = 0.002$, $t = 0.005$ and $t = 0.1$, corresponding to $w = 0$.

The approximate solutions $v^i$ at different time levels and different values of $w$ are plotted in Figures 2-4.

4. CONCLUSIONS

As a novelty of this work we refer to the numerical scheme introduced by (9) in order to approximate the solution to the nonlocal reaction-diffusion problem (1) in presence of the cubic nonlinearity $f(v(t,x)) = v(t,x) - v^3(t,x)$. Corresponding, we have considered an IMEX scheme and in the numerical experiments we focus our attention on a particular case of (1) - the Allen-Cahn...
Fig. 2. The approximate solutions $v^i$ at different levels of time and $w = 5$

Fig. 3. The approximate solutions $v^i$ at different levels of time and $w = -5$
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Fig. 4. The approximate solutions $v^i$ at different levels of time and $w = 10$

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 (12), 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 $\Omega$ at the time $t \in (0, T]$, for example), we found that the instability disappeared from the whole region (see Figures 2-4 for the time level $M = 101$). In addition, 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).

Not least, let’s point out (as an open problem) that the approximate solutions obtained by implementing the numerical algorithm Nonloc-Newton1D can be regarded as admissible for the corresponding boundary optimal control problem.

References


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