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Numerical methods for the generalized Fisher–Kolmogorov–Petrovskii–Piskunov equation ☆

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Abstract

In this paper we study numerical methods for solving integro-differential equations which generalize the well-known Fisher equation. The numerical methods are obtained considering the MOL (Method of Lines) approach. The stability and convergence of the methods are studied. Numerical results illustrating the theoretical results proved are also included.
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1. Introduction

It is well known that the diffusion approximation—Fick's law—to model reaction–diffusion problems gives rise to the Fisher equation

$$\frac{\partial u}{\partial t}(x,t) = D\frac{\partial^2 u}{\partial x^2}(x,t) + f\big(u(x,t)\big), \quad x \in (a,b),\ t > 0. \tag{1}$$

In a large number of biological and chemical phenomena, the reaction term is represented by $f(u) = U(1-u)u$, where $U > 0$ can be dependent of the space variable. Such an equation has the steady state solutions $u = 0$ and $u = 1$, the first one being unstable and the second one stable. The solution of this problem evolves into a traveling wave solution connecting the two steady states with a speed of propagation $c = \sqrt{4DU}$ [1]. When the reaction is very fast, c becomes arbitrarily large. This unphysical property can be corrected if memory effects are taken into account in the mathematical model. This leads to integro-differential equations of type

$$\frac{\partial u}{\partial t}(x,t) = \frac{D}{\tau}\int_0^t e^{-\frac{t-s}{\tau}}\frac{\partial^2 u}{\partial x^2}(x,s)\,\mathrm{d}s + f\big(u(x,t)\big), \quad x \in (a,b),\ t > 0, \tag{2}$$

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with $D \geqslant 0, \tau > 0$, which have been studied for instance in [3–5]. Eq. (2) is known as a generalized Fisher–Kolmogorov–Petrovskii–Piskunov equation, FKPP, and it is coupled with initial and boundary conditions of type

$$u(x,0) = u_0(x), \quad x \in (a,b), \qquad u(a,t) = u_a(t), \quad u(b,t) = u_b(t), \quad t > 0. \tag{3}$$

The parameter τ is a relaxation parameter and when $\tau \to 0$, the FKPP equation is replaced by (1). The existence and the behavior of solutions of Eq. (2) with $f(u) = Uu(1-u)$, $U > 0$, and a Heaviside initial condition was considered in [3]. Different models presenting traveling wave solutions with finite speed of propagation were considered in [6–8].

In this paper we study properties of a class of numerical methods that approximate (2)–(3). In Section 2 we establish an energy estimate that improves the information given by the classical estimate known for the Fisher equation. This new estimate enables us to conclude the stability of (2) relative to perturbations in the initial condition. In Section 3 we use the MOL approach to solve (2)–(3) numerically by using a numerical approximation obtained combining the spatial discretization with a time integration method. A semi-discrete analogue of the estimate established for the theoretical model is deduced for the semi-discrete approximation. In Section 4 fully discrete schemes are analyzed and a discrete version of the continuous estimate is proved, see Theorem 6. As a consequence of Theorem 6 the stability and the convergence of discrete schemes are also studied. Numerical experiments illustrating the theoretical results are presented in Section 5.

2. Energy estimates for the PDE

In this section we study the stability of the solution of (2)–(3) when the initial condition is perturbed. Attending to this fact we assume in Theorem 1 homogeneous Dirichlet boundary conditions. These conditions are considered nonhomogeneous in the rest of the section.

Let $(\cdot,\cdot)$ denote the inner product in $L^2(a,b)$ and $\|\cdot\|_{L^2}$ the usual norm induced by $(\cdot,\cdot)$. If v is defined in $[a,b] \times [0,T]$ we represent $v(\cdot,t)$ by $v(t)$.

We establish in what follows an estimate for the energy functional

$$E(u)(t) = \|u(t)\|_{L^2}^2 + \frac{D}{\tau}\left\| \int_0^t e^{-\frac{t-s}{\tau}} \frac{\partial u}{\partial x}(s)\,\mathrm{d}s \right\|_{L^2}^2, \quad t \in (0,T]. \tag{4}$$

Theorem 1. *Let u be a solution of* (2)–(3) *with $u_a(t) = u_b(t) = 0$, $t > 0$, satisfying for each $t \in [0,T]$*

$$u(x,t) \in [c,d], \quad x \in [a,b], \tag{5}$$

$$\frac{\partial u}{\partial t}(t), \quad \int_0^t e^{-\frac{t-s}{\tau}} \frac{\partial u}{\partial x}(s)\,\mathrm{d}s \in L^2[a,b], \tag{6}$$

where c, d are constants.

If f is continuously differentiable and $f(0) = 0$, then the energy $E(u)$ is such that

$$E(u)(t) \leqslant e^{2\max\{-\frac{1}{\tau}, f'_{\max}\}t} \|u_0\|_{L^2}^2 \tag{7}$$

for each $t \in (0,T]$, where $f'_{\max} = \max_{|u| \leqslant \max\{|c|,|d|\}} f'(u)$.

Proof. Multiplying each member of (2) by u with respect to $(\cdot,\cdot)$ and integrating by parts we obtain

$$\left(\frac{\partial u}{\partial t}(t), u(t)\right) + \frac{D}{\tau}\left(\int_0^t e^{-\frac{t-s}{\tau}} \frac{\partial u}{\partial x}(s)\,\mathrm{d}s, \frac{\partial u}{\partial x}(t)\right) = \big(f\big(u(t)\big), u(t)\big).$$

Considering that

$$\frac{\mathrm{d}}{\mathrm{d}t}\|u(t)\|_{L^2}^2 = 2\left(\frac{\partial u}{\partial t}(t), u(t)\right),$$

and that

$$\frac{d}{dt}\left\|\int_0^t e^{-\frac{t-s}{\tau}}\frac{\partial u}{\partial x}(s)\,ds\right\|_{L^2}^2 = 2\left(\int_0^t e^{-\frac{t-s}{\tau}}\frac{\partial u}{\partial x}(s)\,ds, \frac{\partial u}{\partial x}(\cdot,t)\right) - \frac{2}{\tau}\left\|\int_0^t e^{-\frac{t-s}{\tau}}\frac{\partial u}{\partial x}(s)\,ds\right\|_{L^2}^2,$$

we deduce

$$\frac{d}{dt}\left(\|u(t)\|_{L^2}^2 + \frac{D}{\tau}\left\|\int_0^t e^{-\frac{t-s}{\tau}}\frac{\partial u}{\partial x}(s)\,ds\right\|_{L^2}^2\right) = -\frac{2}{\tau}\frac{D}{\tau}\left\|\int_0^t e^{-\frac{t-s}{\tau}}\frac{\partial u}{\partial x}(s)\,ds\right\|_{L^2}^2 + 2\big(f\big(u(t)\big), u(t)\big). \tag{8}$$

Due to the fact that $f(0)=0$, we have $(f(u(t)), u(t)) \leqslant f'_{\max}\|u(t)\|_{L^2}$ and then from (8), we conclude the differential inequality

$$\frac{d}{dt}E(u)(t) \leqslant 2\max\left\{-\frac{1}{\tau}, f'_{\max}\right\}E(u)(t). \tag{9}$$

Integrating (9) we finally establish (7). □

Under the assumptions of Theorem 1, if (2)–(3) has a solution u then u is unique. Moreover u satisfies

$$\big\|u(t)\big\|_{L^2} \leqslant e^{\max\{-\frac{1}{\tau}, f'_{\max}\}t}\|u_0\|_{L^2}, \tag{10}$$

and

$$\frac{D}{\tau}\left\|\int_0^t e^{-\frac{t-s}{\tau}}\frac{\partial u}{\partial x}(s)\,ds\right\|_{L^2} \leqslant e^{\max\{-\frac{1}{\tau}, f'_{\max}\}t}\|u_0\|_{L^2}. \tag{11}$$

Let us consider now the classical Fisher equation (1). It can be shown that

$$\big\|u(t)\big\|_{L^2} \leqslant e^{f'_{\max}t}\|u_0\|_{L^2} \tag{12}$$

and no information is available about $\frac{\partial u}{\partial x}$. But if u represents the solution of (2), we conclude from (11) that the "average in time" of its gradient is bounded by

$$e^{\max\{-\frac{1}{\tau}, f'_{\max}\}t}\|u_0\|_{L^2},$$

for each time $t \in (0, T]$.

In what follows the stability behavior of u under perturbations in the initial condition u_0 is considered. Let u and u_ε be solutions of (2) satisfying the same boundary conditions (not necessarily homogeneous) and initial conditions u_0 and $u_0+\varepsilon$ respectively. Then $u-u_\varepsilon$, is a solution of the initial-boundary value problem

$$\begin{cases} \frac{\partial}{\partial t}(u-u_\varepsilon)(x,t) = \frac{D}{\tau}\int_0^t e^{-\frac{t-s}{\tau}}\frac{\partial^2}{\partial x^2}(u-u_\varepsilon)(x,s)\,ds + f(u(x,t)) - f(u_\varepsilon(x,t)), & x\in(a,b),\ t\in(0,T], \\ (u-u_\varepsilon)(x,0) = -\varepsilon(x), & x\in(a,b), \\ (u-u_\varepsilon)(a,t) = (u-u_\varepsilon)(b,t) = 0, & t>0. \end{cases} \tag{13}$$

The following stability result can be stated:

Theorem 2. *Let u and u_ε be solutions of* (2)–(3) *with initial conditions u_0 and $u_0+\varepsilon$, respectively. If for u, u_ε* (5) *and* (6) *hold and the source function f is continuously differentiable and $f(0)=0$, then*

$$E(u-u_\varepsilon)(t) \leqslant e^{2\max\{-\frac{1}{\tau}, f'_{\max}\}t}\|\varepsilon\|_{L^2}^2. \tag{14}$$

Proof. Multiplying each member of (13) by $v_\varepsilon = u-u_\varepsilon$ with respect to the inner product $(\cdot,\cdot)$ we obtain

$$\left(\frac{\partial v_\varepsilon}{\partial t}(t), v_\varepsilon(t)\right) + \frac{D}{\tau}\left(\int_0^t e^{-\frac{t-s}{\tau}}\frac{\partial v_\varepsilon}{\partial x}(s)\,ds, \frac{\partial v_\varepsilon}{\partial x}(t)\right) = \big(f\big(u(t)\big) - f\big(u_\varepsilon(t)\big), v_\varepsilon(t)\big).$$

As $(f(u)-f(u_\varepsilon), v_\varepsilon) \leqslant f'_{\max}\|v_\varepsilon\|_{L^2}^2$ following the proof of Theorem 1 we conclude (14). □

In the main result of this section, Theorem 2, we establish the stability of the initial-boundary value problem (2)–(3) with respect to perturbations of the initial condition.

In the case of $f(u) = U(1-u)u$ with $U > 0$, we have $f'_{\max} = U > 0$ and (14) enables us to conclude that for each t, the first member is bounded. If $f'_{\max} < 0$, we obtain

$$\lim_{t\to+\infty}\big\|(u-u_\varepsilon)(t)\big\|_{L^2} = 0, \qquad \lim_{t\to+\infty}\left\|\int_0^t e^{-\frac{t-s}{\tau}}\frac{\partial}{\partial x}(u-u_\varepsilon)(s)\,\mathrm{d}s\right\|_{L^2} = 0.$$

3. Energy estimates for the semi-discrete approximation

In this section we consider the MOL approach to compute a semi-discrete numerical approximation $u_h(t)$ to the solution u of (2)–(3). The approximation $u_h(t)$ is defined by introducing a discretization of the spatial variable. Our aim is to establish a semi-discrete analogue of Theorems 1 and 2 for $u_h(t)$ defined by (15)–(16).

Let us consider in $[a,b]$ a grid $I_h = \{x_j,\ j = 0,\dots,N\}$ with $x_0 = a$, $x_N = b$ and $x_j - x_{j-1} = h$. We discretize the second partial derivative of u with respect to x in (2) using the second-order centered finite-difference operator $D_{2,x}$ defined by

$$D_{2,x}v_h(x_i) = \frac{v_h(x_{i+1}) - 2v_h(x_i) + v_h(x_{i-1})}{h^2}.$$

The semi-discrete approximation $u_h(t)$ is a solution of the following system of ODE's

$$\frac{\mathrm{d}u_h}{\mathrm{d}t}(t) = Au_h(t), \quad t \in (0,T], \tag{15}$$

where

$$\big(Au_h(t)\big)_i = \frac{D}{\tau}\int_0^t e^{-\frac{t-s}{\tau}} D_{2,x}u_h(x_i,s)\,\mathrm{d}s + f\big(u_h(x_i,t)\big), \quad i = 1,\dots,N-1,$$

and

$$u_h(x_0,t) = u_a(t), \qquad u_h(x_N,t) = u_b(t), \qquad u_h(x_i,0) = u_0(x_i), \quad i = 1,\dots,N-1. \tag{16}$$

We denote by $L^2(I_h)$ the space of grid functions v_h defined in I_h such that $v_h(x_0) = v_h(x_N) = 0$. In $L^2(I_h)$ we consider the discrete inner product

$$(v_h,w_h)_h = h\sum_{i=1}^{N-1} v_h(x_i)w_h(x_i), \quad v_h, w_h \in L^2(I_h). \tag{17}$$

We denote by $\|\cdot\|_{L^2(I_h)}$ the norm induced by the above inner product. For grid functions w_h and v_h defined in I_h we introduce the notations

$$(w_h,v_h)_{h,+} = \sum_{i=1}^{N} h w_h(x_i)v_h(x_i),$$

and

$$\|w_h\|_{L^2(I_h^+)} = \left(\sum_{i=1}^{N} h w_h(x_i)^2\right)^{1/2}.$$

Let

$$\|v_h\|_1 = \big(\|v_h\|^2_{L^2(I_h)} + \|D_{-x}v_h\|^2_{L^2(I_h^+)}\big)^{1/2}, \quad v_h \in L^2(I_h),$$

where D_{-x} denotes the backward finite-difference operator. We note that it represents a norm which can be viewed as a discretization of the Sobolev norm of the space $H^1(a,b)$.

Let $E(u_h)(t)$ be the semi-discrete version of $E(u)(t)$ defined by

$$E(u_h)(t) = \|u_h(t)\|^2_{L^2(I_h)} + \frac{D}{\tau}\left\|\int_0^t e^{-\frac{t-s}{\tau}} D_{-x}u_h(s)\,ds\right\|^2_{L^2(I_h^+)}, \quad t > 0.$$

A semi-discrete analogue of Theorem 1 is then established in Theorem 3.

Theorem 3. *Let $u_h(t)$ be a solution of* (15)–(16) *with $u_a(t) = u_b(t) = 0$, $t > 0$, and such that $u_h(x_i, t) \in [c, d]$, for $i = 0, \ldots, N$, and $t \in [0, T]$. If the source function f is continuously differentiable and $f(0) = 0$, then for the energy $E(u_h)(t)$ holds, for each time t in* $(0, T]$,

$$E(u_h)(t) \leqslant e^{2\max\{-\frac{1}{\tau}, f'_{\max}\}t}\|u_0\|^2_{L^2(I_h)}. \tag{18}$$

Proof. Multiplying each member of (15) by $u_h(t)$ with respect to the inner product $(\cdot,\cdot)_h$ and using summation by parts we obtain

$$\frac{1}{2}\frac{d}{dt}\|u_h(t)\|^2_{L^2} + \frac{D}{\tau}\left(\int_0^t e^{-\frac{t-s}{\tau}} D_{-x}u_h(s)\,ds, D_{-x}u_h(t)\right)_{h,+} = \big(f\big(u_h(t)\big), u_h(t)\big)_h,$$

where $f(u_h(t))(x_i) = f(u_h(x_i, t))$, $i = 1, \ldots, N-1$.

Adapting the proof of Theorem 1 to the discrete case it can be shown that the last equality is equivalent to

$$\frac{1}{2}\frac{d}{dt}\left(\|u_h(t)\|^2_{L^2(I_h)} + \frac{D}{\tau}\left\|\int_0^t e^{-\frac{t-s}{\tau}} D_{-x}u_h(s)\,ds\right\|^2_{L^2(I_h)}\right)$$
$$= -\frac{D}{\tau^2}\left\|\int_0^t e^{-\frac{t-s}{\tau}} D_{-x}u_h(s)\,ds\right\|^2_{L^2(I_h^+)} + \big(f\big(u_h(t)\big), u_h(t)\big)_h.$$

As $(f(u_h(t)), u_h(t))_h \leqslant f'_{\max}\|u_h(t)\|^2_{L^2(I_h)}$, we easily conclude (18). □

A semi-discrete version of Theorem 2 is stated in the next result:

Theorem 4. *Let $u_h(t)$, $u_{h,\varepsilon}(t)$ be defined by* (15)–(16) *with initial conditions given respectively by $u_h(x_i, 0) = u_0(x_i)$ and $u_{h,\varepsilon}(x_i, 0) = u_0(x_i) + \varepsilon(x_i)$, $i = 0, \ldots, N$. If $u_h(x_i, t), u_{h,\varepsilon}(x_i, t) \in [c, d]$ for $t \in [0, T]$, $i = 0, \ldots, N$, and the source function f is continuously differentiable and $f(0) = 0$, then*

$$E(u_h - u_{h,\varepsilon})(t) \leqslant e^{2\max\{-\frac{1}{\tau}, f'_{\max}\}t}\|\varepsilon\|^2_{L^2(I_h)}. \tag{19}$$

Proof. The difference $v_h(t) = u_h(t) - u_{h,\varepsilon}(t)$ satisfies the following initial-boundary value problem

$$\begin{cases} \frac{dv_h}{dt}(x_i, t) = \frac{D}{\tau}\int_0^t e^{-\frac{t-s}{\tau}} D_{2,x}v_h(x_i, s)\,ds + f(u_h(x_i, t)) - f(u_{h,\varepsilon}(x_i, t)), \quad i = 1, \ldots, N-1, \\ v_h(x_i, 0) = -\varepsilon(x_i), \quad i = 1, \ldots, N-1, \qquad v_h(x_0, t) = v_h(x_N, t) = 0. \end{cases}$$

Replacing in the proof of Theorem 3, $u_h(t)$ by $v_h(t)$ and $(f(u_h(t)), u_h(t))_h$ by $(f(u_h(t)) - f(u_{h,\varepsilon}(t)), u_h(t))_h$ and considering that $(f(u_h(t)) - f(u_{h,\varepsilon}(t)), v_h(t))_h \leqslant f'_{\max}\|v_h(t)\|^2_{L^2(I_h)}$ we conclude the proof. □

In Theorem 4 the stability of the semi-discrete approximation (15)–(16) is established. In what follows we study the accuracy of $u_h(t)$. Let $T_h(t)$ be the truncation error associated with the spatial discretization defined by (15) and let $e_h(x_i, t) = u(x_i, t) - u_h(x_i, t)$, $i = 0, \ldots, N$, be the spatial discretization error. We have

$$\frac{de_h}{dt}(x_i, t) = \frac{D}{\tau}\int_0^t e^{-\frac{t-s}{\tau}} D_{2,x}e_h(x_i, s)\,ds + f\big(u(x_i, t)\big) - f\big(u_h(x_i, t)\big) + \widetilde{T}_h(x_i, t), \quad i = 1, \ldots, N-1,$$

and

$$e_h(x_0,t)=e_h(x_N,t)=0, \qquad e_h(x_i,0)=0, \quad i=1,\dots,N-1,$$

with $\widetilde{T}_h(x_i,t)=\frac{D}{\tau}\int_0^t e^{-\frac{t-s}{\tau}}T_h(x_i,s)\,\mathrm{d}s$.

For the semi-discretization error $e_h(t)$ holds the following result:

Theorem 5. *Let $u_h(t)$ be the solution of* (15)–(16) *such that $u_h(x_i,t)\in[c,d]$ for $t\in[0,T]$, $i=0,\dots,N$. If the solution u of* (2)–(3) *satisfies* (5) *and the source function f is continuously differentiable and $f(0)=0$, then the spatial discretization error satisfies*

$$E(e_h)(t)\leqslant\frac{D^2}{\tau^2}\int_0^t e^{\max\{-\frac{2}{\tau},2f'_{\max}+1\}(t-s)}\int_0^s \left\|T_h(\mu)\right\|^2_{L^2(I_h)}\,\mathrm{d}\mu\,\mathrm{d}s. \tag{20}$$

Proof. Following the proof of Theorem 3 it can be shown that

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}E(e_h)(t)\leqslant-\frac{D}{\tau^2}\left\|\int_0^t e^{-\frac{t-s}{\tau}}D_{-x}e_h(s)\,\mathrm{d}s\right\|^2_{L^2(I_h^+)}+f'_{\max}\left\|e_h(t)\right\|^2_{L^2(I_h)}+\frac{1}{2}\left\|\widetilde{T}_h(t)\right\|^2_{L^2(I_h)}+\frac{1}{2}\left\|e_h(t)\right\|^2_{L^2(I_h)}.$$

From the last inequality we obtain

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}E(e_h)(t)\leqslant\max\left\{-\frac{1}{\tau},f'_{\max}+\frac{1}{2}\right\}E(e_h)(t)+\frac{1}{2}\left\|\widetilde{T}_h(t)\right\|^2_{L^2(I_h)},$$

that is,

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(e^{-2\max\{-\frac{1}{\tau},f'_{\max}+\frac{1}{2}\}t}E(e_h)(t)-\int_0^t e^{-2\max\{-\frac{1}{\tau},f'_{\max}+\frac{1}{2}\}s}\left\|\widetilde{T}_h(s)\right\|^2_{L^2(I_h)}\,\mathrm{d}s\right)\leqslant 0. \tag{21}$$

Finally, as

$$\left\|\widetilde{T}_h(s)\right\|^2_{L^2(I_h)}\leqslant\frac{D^2}{\tau^2}\int_0^s\left\|T_h(\mu)\right\|^2_{L^2(I_h)}\,\mathrm{d}\mu,$$

we conclude (20) from (21). □

Considering that the spatial discretization is defined using the operator $D_{2,x}$, the truncation error satisfies

$$\left\|T_h(t)\right\|_{L^2(I_h)}\leqslant C\max_{t\in(0,T]}h^2\left\|\frac{\partial^4 u}{\partial x^4}(t)\right\|_\infty=\mathrm{O}\big(h^2\big),$$

where C is a positive constant independent of u and h. Then we conclude that, for each time t,

$$\left\|e_h(t)\right\|^2_{L^2(I_h)}+\frac{D}{\tau}\left\|\int_0^t e^{-\frac{t-s}{\tau}}D_{-x}e_h(s)\right\|^2_{L^2(I_h^+)}\mathrm{d}s=\mathrm{O}\big(h^4\big)$$

and consequently

$$\left\|e_h(t)\right\|_{L^2(I_h)}=\mathrm{O}\big(h^2\big) \tag{22}$$

and

$$\left\|\int_0^t e^{-\frac{t-s}{\tau}}D_{-x}e_h(s)\,\mathrm{d}s\right\|_{L^2(I_h^+)}=\mathrm{O}\big(h^2\big). \tag{23}$$

Being h and t independent variables, we have

$$\|D_{-x}e_h(t)\|_{L^2(I_h^+)} = \mathrm{O}(h^2), \tag{24}$$

which to the best of our knowledge is a nonstandard estimate for the spatial discretization error even when uniform grids are used.

4. Energy estimates for the full discrete approximation

Let us integrate the system of ordinary differential equations (15) using the implicit Euler method in the time grid $\{t_n,\ n = 0, \ldots, M\}$ such that $t_0 = 0,\ t_M = T$ and $t_{n+1} - t_n = \Delta t$. We use the rectangular rule to approximate the integral in (15). The discretization of the reaction could be implicit or explicit depending on the stiffness of the reaction.

In the following we establish an estimate for the fully discrete version of (4),

$$E(u_h^{n+1}) = \|u_h^{n+1}\|^2_{L^2(I_h)} + \frac{D}{\tau}\left\|\Delta t\sum_{\ell=1}^{n+1} e^{-\frac{t_{n+1}-t_j}{\tau}} D_{-x}u_h^{\ell}\right\|^2_{L^2(I_h^+)},$$

where u_h^j is obtained using an implicit or explicit discretization of the reaction term.

1. *Implicit discretization of the reaction term*

In this case the fully discrete approximation of (2) is defined by the nonlinear system of equations

$$\frac{u_h^{n+1}(x_j) - u_h^n(x_j)}{\Delta t} = \frac{D}{\tau}\Delta t\sum_{\ell=1}^{n+1} e^{-\frac{t_{n+1}-t_\ell}{\tau}} D_{2,x}u_h^{\ell}(x_j) + f(u_h^{n+1}(x_j)), \quad j = 1, \ldots, N-1, \tag{25}$$

where

$$u_h^{\ell}(x_0) = u_a(t_\ell), \quad u_h^{\ell}(x_N) = u_b(t_\ell), \quad \ell = 1, \ldots, M-1, \qquad u_h^0(x_j) = u_0(x_j), \quad j = 1, \ldots, N-1. \tag{26}$$

Theorem 6. *Let u_h^ℓ be defined by* (25)–(26) *with $u_a(t) = u_b(t) = 0,\ t > 0$, such that $u_h^\ell(x_i) \in [c, d]$, for $i = 0, \ldots, N$, and $\ell = 0, \ldots, M$. If the source function f is continuously differentiable and $f(0) = 0$, then*

$$\|u_h^{n+1}\|^2_{L^2(I_h)} + \frac{D}{\tau}\left\|\Delta t\sum_{j=1}^{n+1} e^{-\frac{t_{n+1}-t_j}{\tau}} D_{-x}u_h^{j}\right\|^2_{L^2(I_h^+)} \leqslant \left(\frac{1}{\min\{1, 1 - 2\Delta t f'_{\max}\}}\right)^{n+1} \|u_h^0\|^2_{L^2(I_h)} \tag{27}$$

provided that $1 - 2\Delta t f'_{\max} > 0$.

Proof. (a) *Let us consider in* (25) $n \in \mathbb{N}$. Multiplying each member of (25) by u_h^{n+1} with respect to the inner product $(\cdot,\cdot)_h$ and using summation by parts we obtain

$$(u_h^{n+1}, u_h^{n+1})_h = (u_h^n, u_h^{n+1})_h - \frac{D\Delta t^2}{\tau}\sum_{j=1}^{n+1} e^{-\frac{t_{n+1}-t_j}{\tau}} (D_{-x}u_h^j, D_{-x}u_h^{n+1})_{h,+} + \Delta t(f(u_h^{n+1}), u_h^{n+1})_h. \tag{28}$$

As

$$\begin{aligned}&\sum_{j=1}^{n+1} e^{-\frac{t_{n+1}-t_j}{\tau}} (D_{-x}u_h^j, D_{-x}u_h^{n+1})_{h,+}\\ &\quad = \frac{1}{2}\left\|\sum_{j=1}^{n+1} e^{-\frac{t_{n+1}-t_j}{\tau}} D_{-x}u_h^j\right\|^2_{L^2(I_h^+)} - \frac{1}{2}e^{-2\frac{\Delta t}{\tau}}\left\|\sum_{j=1}^{n} e^{-\frac{t_n-t_j}{\tau}} D_{-x}u_h^j\right\|^2_{L^2(I_h^+)} + \frac{1}{2}\|D_{-x}u_h^{n+1}\|^2_{L^2(I_h^+)},\end{aligned} \tag{29}$$

we have from (28)

$$\begin{aligned}
&\|u_h^{n+1}\|^2_{L^2(I_h)} + \frac{D}{2\tau}\left\|\Delta t\sum_{j=1}^{n+1} e^{-\frac{t_{n+1}-t_j}{\tau}} D_{-x}u_h^j\right\|^2_{L^2(I_h^+)} \\
&\quad = \left(u_h^n, u_h^{n+1}\right)_h + \Delta t\left(f\left(u_h^{n+1}\right), u_h^{n+1}\right)_h + \frac{D}{2\tau}e^{-2\frac{\Delta t}{\tau}}\left\|\Delta t\sum_{j=1}^{n} e^{-\frac{t_n-t_j}{\tau}} D_{-x}u_h^j\right\|^2_{L^2(I_h^+)} \\
&\qquad - \frac{D\Delta t^2}{2\tau}\|D_{-x}u_h^{n+1}\|^2_{L^2(I_h^+)}. \qquad (30)
\end{aligned}$$

Considering in (30) the estimates

$$\left(u_h^n, u_h^{n+1}\right)_h \leqslant \frac{1}{2}\|u_h^{n+1}\|^2_{L^2(I_h)} + \frac{1}{2}\|u_h^n\|^2_{L^2(I_h)}, \qquad \left(f\left(u_h^{n+1}\right), u_h^{n+1}\right)_h \leqslant f'_{\max}\|u_h^{n+1}\|^2_{L^2(I_h)},$$

we conclude

$$\begin{aligned}
&\left(1-2\Delta t f'_{\max}\right)\|u_h^{n+1}\|^2_{L^2(I_h)} + \frac{D}{\tau}\left\|\Delta t\sum_{j=1}^{n+1} e^{-\frac{t_{n+1}-t_j}{\tau}} D_{-x}u_h^j\right\|^2_{L^2(I_h^+)} \\
&\quad \leqslant \|u_h^n\|^2_{L^2(I_h)} + \frac{D}{\tau}e^{-2\frac{\Delta t}{\tau}}\left\|\Delta t\sum_{j=1}^{n} e^{-\frac{t_n-t_j}{\tau}} D_{-x}u_h^j\right\|^2_{L^2(I_h^+)}. \qquad (31)
\end{aligned}$$

(b) *We consider now in* (25) $n = 0$. Following the proof of (31) we obtain

$$(1-2\Delta t f'_{\max})\|u_h^1\|^2_{L^2(I_h)} + \frac{D}{\tau}\|\Delta t D_{-x}u_h^1\|^2_{L^2(I_h^+)} \leqslant \|u_h^0\|^2_{L^2(I_h)}. \qquad (32)$$

Finally from (31) and (32) we conclude (27). □

The factor

$$S_I = \frac{1}{\min\{1, 1-2\Delta t f'_{\max}\}}$$

represents the stability amplification factor. If $f'_{\max} < 0$ then $S_I = 1$ and from (27) we obtain

$$\|u_h^{n+1}\|^2_{L^2(I_h)} + \frac{D}{\tau}\left\|\Delta t\sum_{j=1}^{n+1} e^{-\frac{t_{n+1}-t_j}{\tau}} D_{-x}u_h^j\right\|^2_{L^2(I_h^+)} \leqslant \|u_h^0\|^2_{L^2(I_h)}. \qquad (33)$$

Otherwise if $f'_{\max} > 0$, considering that for $\Delta t \leqslant \Delta t_0$ we have

$$S_I = \frac{1}{1-2\Delta t f'_{\max}} = 1 + \frac{2f'_{\max}}{1-2\Delta t f'_{\max}}\Delta t \leqslant 1 + \frac{2f'_{\max}}{1-2\Delta t_0 f'_{\max}}\Delta t,$$

we conclude

$$\|u_h^{n+1}\|^2_{L^2(I_h)} + \frac{D}{\tau}\left\|\Delta t\sum_{j=1}^{n+1} e^{-\frac{t_{n+1}-t_j}{\tau}} D_{-x}u_h^j\right\|^2_{L^2(I_h^+)} \leqslant e^{\beta(n+1)\Delta t}\|u_h^0\|^2_{L^2(I_h)} \qquad (34)$$

with

$$\beta = \frac{2f'_{\max}}{1-2\Delta t_0 f'_{\max}}.$$

2. *Explicit discretization of the reaction term*

Let us consider now the IMEX scheme obtained by replacing in (25) $f(u_h^{n+1})$ by $f(u_h^n)$, that is,

$$\frac{u_h^{n+1}(x_j) - u_h^n(x_j)}{\Delta t} = \frac{D}{\tau}\Delta t\sum_{\ell=1}^{n+1} e^{-\frac{t_{n+1}-t_\ell}{\tau}} D_{2,x}u_h^\ell(x_j) + f\left(u_h^n(x_j)\right), \quad j = 1, \ldots, N-1. \qquad (35)$$

We remark that with $\tilde{u}_h^n = \theta u_h^n$ for $\theta \in [0,1]$, we have

$$2\Delta t\big(f\big(u_h^n\big), u_h^{n+1}\big)_h = 2\Delta t\big(f'\big(\tilde{u}_h^n\big)u_h^n, u_h^{n+1}\big)_h \leqslant \Delta t\big\|u_h^n\big\|_{L^2(I_h)}^2 + \Delta t(f'_{\max})^2\big\|u_h^{n+1}\big\|_{L^2(I_h)}^2.$$

Then the stability coefficient S_I is replaced by the stability coefficient S_{IMEX} defined by

$$S_{IMEX} = \frac{1+\Delta t}{1-\Delta t(f'_{\max})^2}$$

provided that $1-\Delta t(f'_{\max})^2 > 0$. We have

$$S_{IMEX} \leqslant 1 + \frac{1+(f'_{\max})^2}{1-\Delta t_0(f'_{\max})^2}\Delta t$$

and we can prove (34) with

$$\beta = \frac{1+(f'_{\max})^2}{1-\Delta t_0(f'_{\max})^2}.$$

Let us study now the convergence of the approximation defined by (25), (26). Let $e_h^\ell(x_i) = u_h^\ell(x_i) - u(x_i, t_\ell)$ be the global error of the approximation $u_h^\ell(x_i)$ computed using (25), (26), and let $T_h^\ell(x_i)$ be the corresponding truncation error. These two errors are related by

$$e_h^{n+1}(x_i) = e_h^n(x_i) + \frac{D}{\tau}\Delta t^2\sum_{j=1}^{n+1} e^{-\frac{t_{n+1}-t_j}{\tau}} D_{2,x}e_h^j(x_i)$$
$$+ f\big(u_h^{n+1}(x_i)\big) - f\big(u(x_i, t_{n+1})\big) + \Delta t T_h^{n+1}(x_i), \quad i = 1,\ldots,M-1 \tag{36}$$

with

$$e_h^0(x_i) = 0, \quad i = 1,\ldots,N-1, \qquad e_h^\ell(x_0) = e_h^\ell(x_N) = 0, \quad \ell = 1,\ldots,M.$$

Following the proof of Theorem 6 the next convergence result can be proved.

Theorem 7. *Let u_h^ℓ be defined by* (25)–(26) *and such that $u_h^\ell(x_i) \in [c,d]$, for all i and for all ℓ. If the solution u of* (2)–(3) *satisfies* (5) *and the source function f is continuously differentiable and $f(0) = 0$, then*

$$\big\|e_h^{n+1}\big\|_{L^2(I_h)}^2 + \frac{D}{\tau}\left\|\Delta t\sum_{j=1}^{n+1} e^{-\frac{t_{n+1}-t_j}{\tau}} D_{-x}e_h^j\right\|_{L^2(I_h^+)}^2 \leqslant \sum_{j=0}^{n}\widehat{S}_I^{j+1}\Delta t\big\|T_h^{n+1-j}\big\|_{L^2(I_h)}^2 \tag{37}$$

with

$$\widehat{S}_I = \frac{1}{\min\{1, 1-(1+2f'_{\max})\Delta t\}}.$$

Considering that (25) is defined approximating the second-order spatial derivative using centered differences, the integral term using the rectangular rule and the integration in time using the Euler implicit method, we have

$$T_h^{n+1}(x_i) = -\frac{\Delta t}{2}\frac{\partial^2 u}{\partial t^2}(x_i, t_n^*) - \frac{D}{\tau}\sum_{j=1}^{n+1}\int_{t_{j-1}}^{t_j}\frac{\partial}{\partial s}\left(e^{-\frac{t_{n+1}-s}{\tau}}\frac{\partial^2 u}{\partial x^2}(x_i, s)\right)(s - t_{j+1})\,\mathrm{d}s$$
$$- \frac{h^2}{24}\frac{D}{\tau}\Delta t\sum_{j=1}^{n+1} e^{-\frac{t_{n+1}-t_j}{\tau}}\left(\frac{\partial^4 u}{\partial x^4}(x_i^*, t_j) + \frac{\partial^4 u}{\partial x^4}(\bar{x}_i, t_j)\right),$$

where $t_n^* \in [t_n, t_{n+1}]$, $x_i^*, \bar{x}_i \in [x_{i-1}, x_{i+1}]$. Then

$$\|T_h\|_\infty = \max_\ell \|T_h^\ell\|_\infty \leqslant C \max_{t\in(0,T]} \left(\Delta t\left(\left\|\frac{\partial^2 u}{\partial t^2}(t)\right\|_\infty + \left\|\frac{\partial^2 u}{\partial x^2}(t)\right\|_\infty + \left\|\frac{\partial^3 u}{\partial t\partial x^2}(t)\right\|_\infty\right) + h^2\left\|\frac{\partial^4 u}{\partial x^4}(t)\right\|_\infty\right). \tag{38}$$

In the last inequality C denotes a generic positive constant independent of h, Δt and u. Using (38) in Theorem 7 we conclude:

Corollary 1. *Under the assumptions of Theorem 7 and assuming $f'_{\max} \leqslant -\frac{1}{2}$ then*

$$\|e_h^n\|^2_{L^2(I_h)} + \frac{D}{\tau}\left\|\Delta t \sum_{j=1}^n e^{-\frac{t_n - t_j}{\tau}} D_{-x} e_h^j\right\|^2_{L^2(I_h^+)} \leqslant C\|T_h\|^2_\infty. \tag{39}$$

If $f'_{\max} > -\frac{1}{2}$ then

$$\|e_h^n\|^2_{L^2(I_h)} + \frac{D}{\tau}\left\|\Delta t \sum_{j=1}^n e^{-\frac{t_n - t_j}{\tau}} D_{-x} e_h^j\right\|^2_{L^2(I_h^+)} \leqslant C e^{\beta n \Delta t}\|T_h\|^2_\infty, \tag{40}$$

with

$$\beta = \frac{1 + 2f'_{\max}}{1 - (1 + 2f'_{\max})\Delta t_0}.$$

Analogous convergence results can be established for the IMEX method.

5. Numerical results

In this section we present some numerical results that show the effectiveness of the estimates presented in Theorems 5 and 7.

5.1. A semi-discrete approximation

Let us consider the semi-discrete system of ordinary differential equations (15). In order to avoid the integral term and as our aim is to illustrate the behavior of the spatial discretization we rewrite (15) in the following form

$$\begin{cases} \frac{dv_h}{dt}(x_i, t) = -\frac{1}{\tau} v_h(x_i, t) + u_h(x_i, t), & i = 1, \dots, N-1, \\ \frac{du_h}{dt}(x_i, t) = \frac{D}{\tau} D_{2,x} v_h(x_i, t) + f(u_h(x_i, t)), & i = 1, \dots, N-1, \end{cases} \tag{41}$$

with the initial boundary conditions

$$\begin{cases} v_h(x_i, 0) = 0, & i = 1, \dots, N-1, \\ v_h(x_i, t) = \int_0^t e^{-\frac{t-s}{\tau}} u_h(x_i, s)\, ds, & i = 0, N, \\ u_h(x_0, t) = u_a(t), & u_h(x_N, t) = u_b(t), \\ u_h(x_i, 0) = u_0(x_i), & i = 1, \dots, N-1. \end{cases} \tag{42}$$

To illustrate the second-order estimates in space (22) and (24) we integrate in time (41) with a fourth-order Runge–Kutta method. The numerical results obtained with $u_0(x) = e^{-(x-25)^2}$, $x \in [0, 50]$, $f(u) = Uu(1-u)$, $U = 1$, $D = 0.2$, $\tau = 0.1$ and $\Delta t = 0.05$ are presented in Table 1. The estimates for the orders p and p^* exhibited in this table were computed using

$$p = \frac{\log\left(\frac{\max_{j=0,\dots,M} \|e_{h_1}^j\|_{L^2(I_{h_1})}}{\max_{j=0,\dots,M} \|e_{h_2}^j\|_{L^2(I_{h_2})}}\right)}{\log\left(\frac{h_1}{h_2}\right)} \quad \text{and} \quad p^* = \frac{\log\left(\frac{\max_{j=0,\dots,M} \|D_{-x} e_{h_1}^j\|_{L^2(I_{h_1}^+)}}{\max_{j=0,\dots,M} \|D_{-x} e_{h_2}^j\|_{L^2(I_{h_2}^+)}}\right)}{\log\left(\frac{h_1}{h_2}\right)},$$

respectively, where h_1 and h_2 represent different space step-sizes. We considered $M = 500$ and the error was estimated using a reference solution computed with $\Delta t = 0.01$, $h = 0.025$.

Table 1

h	0.1	0.2	0.3	0.4	0.5	0.6
p	2.0706	2.0222	2.0114	2.0067	2.0140	
p^*	2.0568	1.9829	1.9337	1.8870	1.8409	

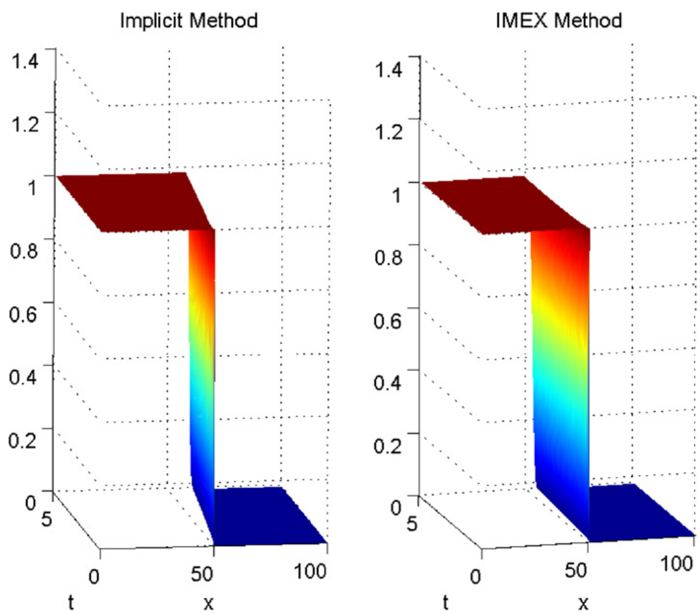

Fig. 1. Numerical solutions computed with methods (25) and (35) for $U = 1$, $\tau = D = 0.1$ and $\Delta t = h = 0.1$.

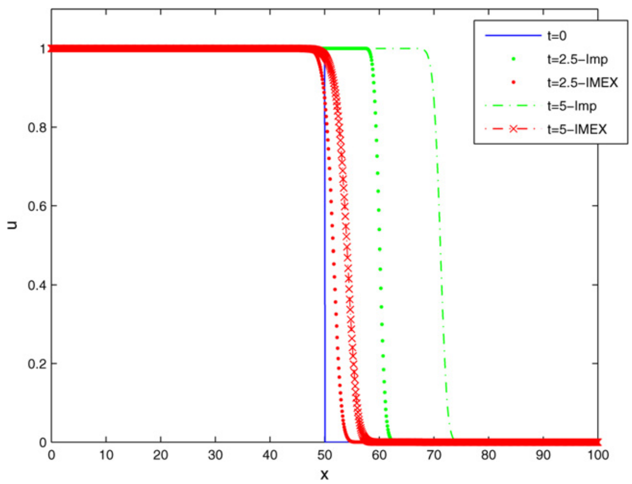

Fig. 2. Numerical solutions computed with methods (25) and (35) for $U = 1$, $\tau = D = 0.1$ and $\Delta t = h = 0.1$.

5.2. A fully discrete approximation

We present in what follows some numerical results that illustrate the qualitative and stability properties of methods (25) and (35). The computational experiments have been obtained with a reaction term of type $f(u) = U(1-u)u$, and with the initial condition

$$u_0(x) = \begin{cases} 1, & x \in [0, 50], \\ 0, & x \in]50, 100]. \end{cases}$$

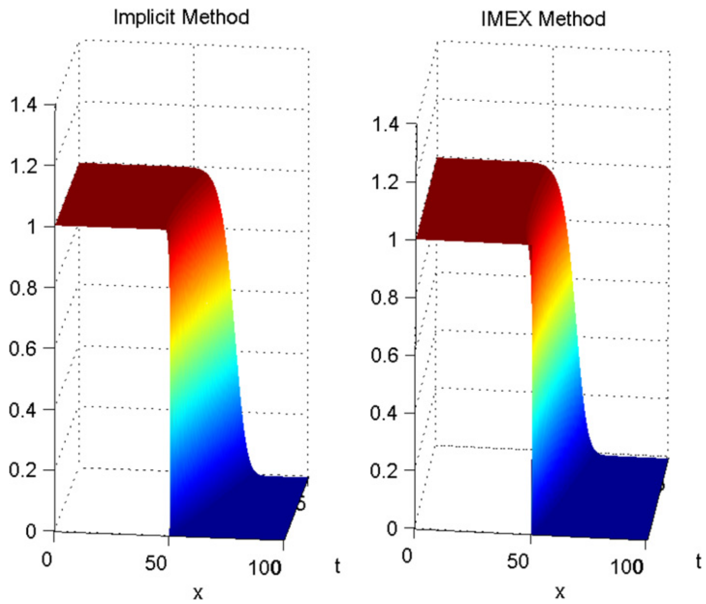

Fig. 3. Numerical solutions computed with methods (25) and (35) for $U = 1$, $\tau = 0.1$, $\Delta t = h = 0.1$ and $D = 2$.

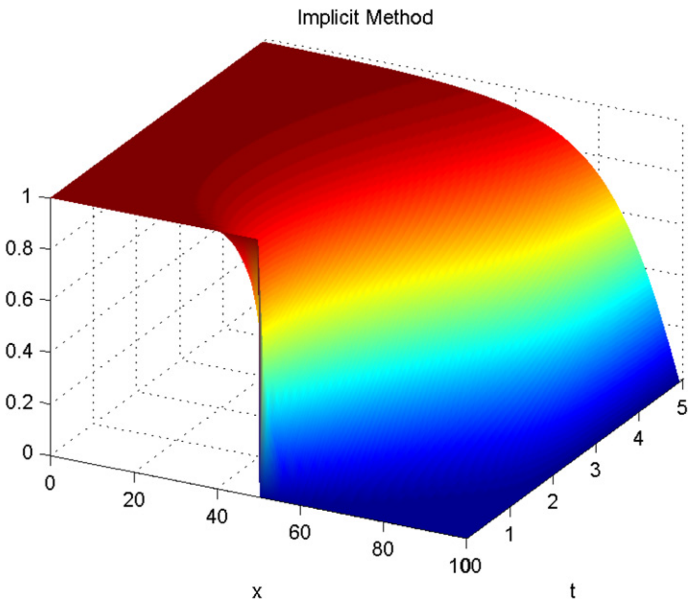

Fig. 4. Numerical solution computed with method (25) for $U = 1$, $D = 0.1$, $\Delta t = h = 0.1$ and $\tau = 0.001$.

In Fig. 1 we plot the numerical approximations obtained using method (25) and method (35) with $U = 1$, $\tau = 0.1 = D = 0.1$ and $\Delta t = h = 0.1$. The two numerical solutions exhibit the same stability behavior, but as we can see in Fig. 2 the speed of the numerical solution obtained with method (25) is greater.

In Fig. 3 we plot the numerical approximations obtained for $D = 2$. As expected, we observe in Figs. 1 and 3 that increasing diffusion leads to a smoother solution.

The numerical approximation obtained from (25) with $D = 1$ and $\tau = 0.001$ is plotted in Fig. 4. The plots presented in Figs. 2 and 4 illustrate the fact that the generalized FKPP equation is replaced by the classical Fisher equation when $\tau \to 0$.

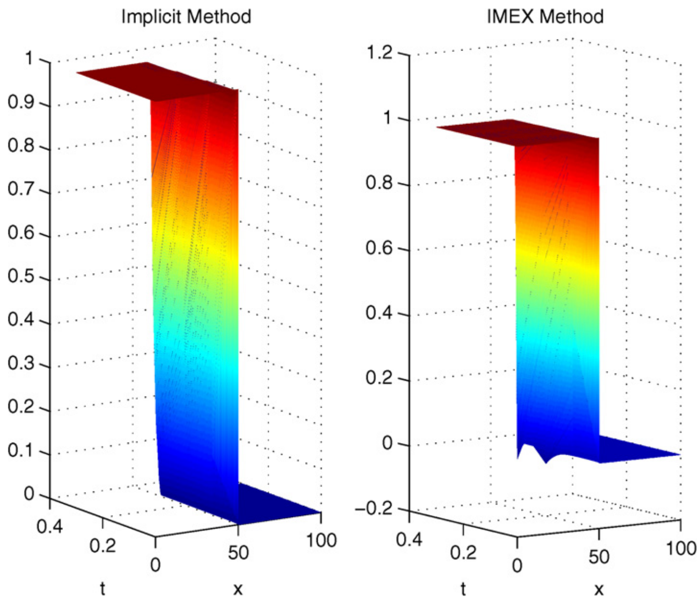

Fig. 5. Numerical solutions computed with methods (25) and (35) for $D = \tau = 0.1 = \Delta t = h = 0.1$ and $U = -25$.

We have shown in Section 4 that if the reaction term f is stiff, then method (25) is more stable then method (35). This behavior is illustrated in Fig. 5 where we plot the numerical solution obtained with the previous methods for $U = -25$ and $h = \Delta t = \tau = D = 0.1$. As can be observed, the numerical solution obtained with method (35) presents an unstable behavior.

Finally we remark that when time t increases the discretization of the integral term needs more and more computational memory and the method can become very expensive. In order to avoid this drawback, method (25) can be rewritten in the following equivalent form:

$$\begin{aligned}
&\left(I - \frac{D\Delta t^2}{\tau} D_{2,x}\right) u_h^{n+1}(x_i) - \Delta t f\left(u_h^{n+1}(x_i)\right) \\
&\quad = \left(1 + e^{-\frac{\Delta t}{\tau}}\right) u_h^n(x_i) - \Delta t e^{-\frac{\Delta t}{\tau}} f\left(u_h^n(x_i)\right) - e^{-\frac{\Delta t}{\tau}} u_h^{n-1}(x_i), \quad n = 1, \ldots, M-1, \\
&\left(I - \frac{D\Delta t^2}{\tau} D_{2,x}\right) u_h^1(x_i) - \Delta t f\left(u_h^1(x_i)\right) = u_h^0(x_i).
\end{aligned} \tag{43}$$

Due to the discretization of the memory term the IMEX method (35) can also be computationally expensive. In order to avoid this limitation method (35) can be rewritten in the following equivalent form:

$$\begin{aligned}
&\left(I - \frac{D\Delta t^2}{\tau} D_{2,x}\right) u_h^{n+1}(x_i) \\
&\quad = \left(1 + e^{-\frac{\Delta t}{\tau}}\right) u_h^n(x_i) + \Delta t f\left(u_h^n(x_i)\right) + \Delta t e^{-\frac{\Delta t}{\tau}} f\left(u_h^{n-1}(x_i)\right) - e^{-\frac{\Delta t}{\tau}} u_h^{n-1}(x_i), \quad n = 1, \ldots, M-1, \\
&\left(I - \frac{D\Delta t^2}{\tau} D_{2,x}\right) u_h^1(x_i) = u_i^0 + \Delta t f\left(u_h^0(x_i)\right).
\end{aligned} \tag{44}$$

Finally we remark that in [2], [9] and [10] were considered different methods for equations of type (2).

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