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Numerical analysis of the Caughley model from ecology*,†

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Abstract. This paper deals with numerical analysis of a reaction diffusion model from mathematical ecology posed in an unbounded spatial domain. For numerical simulations we replace the original system with an equivalent one posed in a bounded domain. This is done by means of an algebraic map in conjunction with a spectral method. For the semidiscretization in time we use an exponential time differencing scheme, the resulting scheme is explicit both in space and time. Improved error estimates are derived and the computational efficiency of the algorithm is considered. Finally, we present several numerical simulations which are useful for making pertinent biological deductions.
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1. Introduction

In this paper we deal with the following system of reaction-diffusion equations

$$u_t = a_1\triangle u + u\Big(a - \frac{au}{K} - \frac{cv}{v+g}\Big), \quad u(0) = u_0, \tag{1a}$$

$$v_t = a_2\triangle v + v\Big(-A + \frac{ku}{u+B}\Big), \quad v(0) = v_0, \tag{1b}$$

where $u_0, v_0 \in L^2(\mathbb{R}^d)$ and $\triangle$ is the Laplacian. In mathematical ecology (1) is known as the Caughley model with diffusion [14]. The unknown functions u and v represent densities of trees and elephants, respectively. The reaction terms provide a type II functional response of the system. Equation (1) contains a number of ecological parameters, their meaning are as follows: a — the natural rate of increase, K — the tree carrying capacity, c — the instantaneous elimination rate of tree by elephants, g — the threshold above which tree destruction depends only on the elephants, A — the elephants decrease rate in the absence of trees, k — the ameliorated decrease rate in given ratio of trees to elephants, B — the threshold above which the amelioration depends only on the trees. The major difficulty in the numerical simulation of (1)

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stems from the unboundedness of the spatial domain. The standard solution in this situation is to replace the original system (1) posed on the infinite domain by an equivalent one posed on a bounded domain.

The reduction strategy depends on the aims of the numerical simulation and on the physical nature of the phenomena under investigation. For instance, if one is interested in the solutions of (1) in a bounded subdomain $\Omega \subset \mathbb{R}^n$, then it is natural to introduce artificial (or transparent) boundary conditions (ABC or TBC) on $\partial\Omega$. This technique works well for linear equations when initial data is compactly supported in the interior of Ω. When the asymptotical behaviour of the solution is known a priori the ABC method could be extended to nonlinear equations as well. Another possible approach is based on the fast evaluation of the heat potential. This method is specifically designed to cope with linear equations.

We are interested in the long time behaviour of the complete system (1). As a consequence of that and also due to the nonlinearities involved in the model the techniques based on the domain truncation are not suitable. Better results are obtained if we map $\mathbb{R}^n$ onto a bounded domain and then solve the resulting system numerically. In the present paper we propose an algorithm based on an algebraic map in conjunction with a spectral discretization in space.

The paper is organized as follows: section 2 deals with numerical discretization of (1). The detailed account on the time semidiscretization is provided in subsection 2.1. The analysis of spectral approximations is given in subsection 2.2. In section 3, some aspects of practical computations are addressed. The final section contains the results of numerical simulations.

2. Numerical discretization

To obtain a computational scheme we discretize (1) first in time and then in space.

2.1. Semidiscretization in time

Equation (1) can be viewed as an abstract differential equation of the form $u_t = \mathcal{L}u + f(u)$. In (1) the nonlinear operator $\mathcal{L} + f(\cdot)$ generates a strongly continuous semigroup over $L^2(\mathbb{R}^d)$ for $d \leq 3$, see [14], consequently, the solution can be written as

$$u(t+\tau) = e^{\tau\mathcal{L}}u(t) + \int_0^\tau e^{(t-s)\mathcal{L}} f(u(t+s))ds, \tag{2}$$

where $\tau > 0$ is a stepsize. The simplest semidiscretization in time is obtained if we let $u_k \approx u(k\tau)$ and replace $f(u(k\tau+s))$ with $f(u(k\tau))$ in the integral term of (2)

$$u_{k+1} = e^{\tau\mathcal{L}}u_k + \tau\psi_1(\tau\mathcal{L})f(u_k), \quad k \geq 0, \tag{3}$$

where

$$\psi_0(z) = e^z, \quad \psi_\ell(z) = \frac{1}{(\ell-1)!}\int_0^1 e^{sz}(1-s)^{\ell-1}ds, \quad \ell = 1, 2, \ldots \tag{4}$$

Scheme (3) is known as the Exponential Time Differencing (ETD) Euler method. In general, methods of the form (3) are known as the exponential integrators, a survey on the exponential multistep and Runge-Kutta methods is available in [10]. In our computations we use the exponential five-stage Runge-Kutta scheme of stiff order four developed by Hochbruck and Ostermann [8]

$$u_{k,1} = e^{\frac{\tau}{2}\mathcal{L}}u_k + \frac{\tau}{2}\psi_{1,2}(\tau\mathcal{L})f(u_k), \tag{5a}$$

$$u_{k,2} = e^{\frac{\tau}{2}\mathcal{L}}u_k + \tau\Big[\frac{1}{2}\psi_{1,2} - \psi_{2,2}\Big](\tau\mathcal{L})f(u_k) + \tau\psi_{2,2}(\tau\mathcal{L})f(u_{k,1}), \tag{5b}$$

$$u_{k,3} = e^{\tau\mathcal{L}}u_k + \tau\Big[\psi_1 - 2\psi_2\Big](\tau\mathcal{L})f(u_k) + \tau\psi_2(\tau\mathcal{L})\Big[f(u_{k,1}) + f(u_{k,2})\Big], \tag{5c}$$

$$\begin{aligned} u_{k,4} = {}& e^{\frac{\tau}{2}\mathcal{L}}u_k + \tau\Big[\frac{1}{2}\psi_{1,2} - 2a_{5,2} - a_{5,4}\Big](\tau\mathcal{L})f(u_k) \\ & + \tau a_{5,2}(\tau\mathcal{L})\Big[f(u_{k,1}) + f(u_{k,2})\Big] + \tau a_{5,4}(\tau\mathcal{L})f(u_{k,3}), \end{aligned} \tag{5d}$$

$$\begin{aligned} u_{k+1} = {}& e^{\tau\mathcal{L}}u_k + \tau\Big[\psi_1 - 3\psi_2 + 4\psi_3\Big](\tau\mathcal{L})f(u_k) \\ & + \tau\Big[4\psi_3 - \psi_2\Big](\tau\mathcal{L})f(u_{k,3}) + \tau\Big[4\psi_2 - \psi_3\Big](\tau\mathcal{L})f(u_{k,4}), \end{aligned} \tag{5e}$$

where

$$a_{5,2} = \frac{1}{2}\psi_{2,2} - \psi_3 + \frac{1}{4}\psi_2 - \frac{1}{2}\psi_{3,2}, \quad a_{5,4} = \frac{1}{4}\psi_{2,2} - a_{5,2}, \quad \psi_{\ell,2}(z) = \psi_\ell\Big(\frac{1}{2}z\Big).$$

Semidiscretization (5) converges to the solution of (1) with order four, i.e. $\|u_k - u(k\tau)\|_{L^2(\mathbb{R}^d)} = \mathcal{O}(\tau^4)$, provided that the nonlinearity $f(u)$ is sufficiently smooth and $u_k, u_{k,j}, f(u_k), f(u_{k,j}) \in L^2(\mathbb{R}^d)$, $j = 1, \dots, 5$, $k \geq 0$ are known exactly. In a computational scheme these quantities must be approximated and since the space $L^2(\mathbb{R}^d)$ is separable, it is natural to use a pseudospectral approach. The details are provided in the next subsection.

2.2. Discretization in space

Given a separable Hilbert space H and an orthogonal basis $\{\phi_n\}_{n\geq 0}$, in the spectral (pseudospectral) approach we approximate $f \in H$ by its truncated Fourier series (interpolant). A particular choice of the family $\{\phi_n\}_{n\geq 0}$ depends on the structure of H. In a classical situation, when $H = L^2_w([-1,1])$, $w(x) = (1+x)^\alpha(1-x)^\beta$, the bases are provided by Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$, $n \geq 0$, $\alpha, \beta > -1$. Two cases $\alpha = \beta = -1/2$ (Chebyshev polynomials $T_n(x)$) and $\alpha = \beta = 0$ (Legendre polynomials $P_n(x)$) are of special importance, see [4, 5, 6].

Since we deal with $H = L^2(\mathbb{R}^d)$, the spatial domain is unbounded and as a result the choice of a good family $\{\phi_n\}_{n\geq 0}$ becomes a very delicate issue. We mention that for $d = 1$ the computationally feasible options are: the Hermite functions, the sinc expansion, use of mappings in conjunction with classical Jacobi polynomials, see [4, 5] and references therein. By the reasons discussed in the introduction we employ the last alternative. For the sake of simplicity, we assume that $d = 1$. Let $\ell > 0$ be a parameter, then $y = x/(\sqrt{\ell^2 + x^2})$ maps $\mathbb{R}$ into $[-1, 1]$. As the complete orthogonal basis in $L^2(\mathbb{R})$ we use the following modification of algebraically mapped

Chebyshev polynomials $TB_n(x) = T_n\Big(\dfrac{x}{\sqrt{\ell^2+x^2}}\Big)$ (see [4]):

$$\phi_n(x) = \frac{\sqrt{\ell}}{\sqrt{\ell^2+x^2}} TB_n(x) = \frac{\sqrt{\ell}}{\sqrt{\ell^2+x^2}} \cos(n \operatorname{arccot} x/\ell), \quad n \geq 0. \tag{6}$$

Some approximation properties of (6) can be derived directly from the theory of TB_n, see [4] and references therein. Below we provide new $L^2(\mathbb{R})$ approximation results in the spirit of [9], see also [5]. We found that the analysis simplifies if we work with Fourier images of ϕ_n. Further, we briefly mention some results related to fractional integrodifferentiation and the Fourier transform.

2.2.1. Bessel fractional integroderivatives

Our presentation closely follows [12, pp. 253-256], see also [2, pp. 219-222]. Let $f(x)$ be a function, by $\hat{f}(s)$ or $\mathcal{F}[f](s)$ we denote its normalized Fourier transform $\mathcal{F}[f](s) = \dfrac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} f(x)e^{-isx}dx$. The left and the right Bessel fractional integrals (derivatives) of order α, $\Re\alpha > 0$ ($\Re\alpha \leq 0$) are defined as follows

$$\mathcal{F}[J_{\pm}^{\alpha,q} f](s) = \frac{\hat{f}(s)}{(q \mp is)^{\alpha}}, \quad \text{for some} \quad 0 < q < \infty. \tag{7}$$

The number q is a normalization parameter, it helps to simplify some of our analytical calculations. We mention the following properties of Bessel fractional integrals (7) (see [12, pp. 253-256]): $J_{\pm}^{\alpha,q}$ are bounded linear operators in $L^p(\mathbb{R})$, they satisfy

$$J_{\pm}^{\alpha,q} J_{\pm}^{\beta,q} f = J_{\pm}^{\alpha+\beta,q} f, \quad \Re\alpha, \Re\beta > 0, \quad f \in L^p(\mathbb{R}), \quad 1 \leq p \leq \infty, \tag{8}$$

the family $\{J_{\pm}^{\alpha,q}\}_{\alpha>0}$ generates a continuous semigroup in $L^p(\mathbb{R})$ and the formula of fractional integration by parts

$$\int_{\mathbb{R}} f J_{\pm}^{\alpha,q} g dx = \int_{\mathbb{R}} g J_{\mp}^{\alpha,q} f dx, \quad \Re\alpha > 0, \tag{9}$$

holds, where $f \in L^p(\mathbb{R})$, $g \in L^{(p-1)/p}(\mathbb{R})$, $1 \leq p \leq \infty$. The definition of $J_{\pm}^{\alpha,q}$, $\Re\alpha > 0$ yields

$$\mathcal{F}[J_{\pm}^{\alpha,q} f](s) = \frac{\hat{f}(s)}{(q \mp is)^{\alpha}} \quad \text{and} \quad \mathcal{F}^{-1}[J_{\pm}^{\alpha,q} \hat{f}](x) = \frac{f(x)}{(q \pm ix)^{\alpha}}, \tag{10}$$

where $f \in L^p(\mathbb{R})$, $1 \leq p \leq 2$ and $\hat{f} \in L^{p/(p-1)}(\mathbb{R})$ according to the Hausdorff-Young inequality.

Bessel fractional derivative $J_{\pm}^{-\alpha,q}$ is the left inverse to $J_{\pm}^{\alpha,q}$, $\Re\alpha > 0$, that is $J_{\pm}^{-\alpha,q} J_{\pm}^{\alpha,q} = I$, see [12, pp. 253-256]. The formula of fractional integration by parts takes the form

$$\int_{\mathbb{R}} f J_{\pm}^{-\alpha,q} g dx = \int_{\mathbb{R}} g J_{\mp}^{-\alpha,q} f dx, \tag{11}$$

provided that $f, J_{\pm}^{-\alpha,q} f \in L^p(\mathbb{R})$ and $g, J_{\pm}^{-\alpha,q} g \in L^{p/(p-1)}(\mathbb{R})$ for some $1 \le p \le \infty$. In complete analogy with (10), we have

$$\mathcal{F}[J_{\pm}^{-\alpha,q} f](s) = (q \mp is)^{\alpha} \hat{f}(s) \quad \text{and} \quad \mathcal{F}^{-1}[J_{\pm}^{-\alpha,q} \hat{f}](x) = (q \pm ix)^{\alpha} f(x), \qquad (12)$$

provided that $J_{\pm}^{-\alpha,q} f \in L^p(\mathbb{R})$ and $1 \le p \le 2$.

In the sequel we prove the following analogue of Lemma 3.2 from [12, p. 67]:

Lemma 1. *Let $f \in L^2(\mathbb{R})$ and $\alpha, \beta > 0$, then*

$$\|J_{\pm}^{-\alpha,1}[(1+x^2)^{\beta} f]\|_{L^2(\mathbb{R})} \le c_{\alpha,\beta} \|(1+x^2)^{\beta} J_{\pm}^{-\alpha,1} f\|_{L^2(\mathbb{R})}, \qquad (13)$$

where $c_{\alpha,\beta} > 0$ does not depend on f, provided that $\|(1+x^2)^{\beta} J_{\pm}^{-\alpha,1} f\|_{L^2(\mathbb{R})} < \infty$.

Proof. It is sufficient to prove (13) for $0 < \alpha < 1$ and $0 < \beta \le 1/2$. For the general case we then have

$$c_{\alpha,\beta} = c_{1/2,1/2}^{4\lfloor\beta\rfloor\lfloor\alpha\rfloor} c_{1/2,\{\beta\}}^{2\lfloor\alpha\rfloor} c_{\{\alpha\},1/2}^{2\lfloor\beta\rfloor} c_{\{\alpha\},\{\beta\}}, \quad 0 \le \{\beta\} \le 1/2,$$
$$c_{\alpha,\beta} = c_{1/2,1/2}^{2(2\lfloor\beta\rfloor+1)\lfloor\alpha\rfloor} c_{1/2,\{\beta\}-1/2}^{2\lfloor\alpha\rfloor} c_{\{\alpha\},1/2}^{2\lfloor\beta\rfloor+1} c_{\{\alpha\},\{\beta\}-1/2}, \quad 1/2 < \{\beta\} < 1,$$

where $\alpha = \lfloor\alpha\rfloor + \{\alpha\}$, $\beta = \lfloor\beta\rfloor + \{\beta\}$ and the symbols $\lfloor\alpha\rfloor$, $\lfloor\beta\rfloor$ and $\{\alpha\}$, $\{\beta\}$ denote integer and fractional part of α and β, respectively.

For the sake of brevity, we prove (13) for the left Bessel fractional derivative only, the proof for $J_{-}^{\alpha,1}$ is almost identical. The inequality $\|(1+x^2)^{\beta} J_{+}^{-\alpha,1} f\|_{L^2(\mathbb{R})} < \infty$ implies that there exists $\psi \in L^2(\mathbb{R})$ such that $f = J_{+}^{\alpha,1}[(1+x^2)^{-\beta}\psi]$. We show that $f = (1+x^2)^{-\beta} J_{+}^{\alpha,1}\phi$ for $\phi = \psi + \mathcal{K}\psi \in L^2(\mathbb{R})$, where

$$\mathcal{K}[\psi](x) = \frac{2\beta \sin \pi\alpha}{\pi} \int_{-\infty}^{x} K(x,t)\psi(t)dt, \; K(x,t) = \frac{e^{t-x}}{x-t} \int_{t}^{x} \Big(\frac{y-t}{x-t}\Big)^{\alpha} \frac{y(1+y^2)^{\beta-1}}{(1+t^2)^{\beta}} dy.$$

First, we note that $\mathcal{K}$ is a linear bounded operator in $L^2(\mathbb{R})$. Indeed, the elementary inequality $(1+(a+b)^2)^{\beta} \le (1+a^2)^{\beta} + (1+b^2)^{\beta}$, which holds for all $a, b \in \mathbb{R}$ and $0 \le \beta \le 1/2$, yields the pointwise estimate

$$\begin{aligned}
|\mathcal{K}[\psi](x)| &\le \frac{2\beta \sin \pi\alpha}{\pi} \int_{-\infty}^{x} e^{t-x} |\psi(t)| dt \left| \frac{1}{x-t} \int_{t}^{x} \Big(\frac{y-t}{x-t}\Big)^{\alpha} \frac{y(1+y^2)^{\beta-1}}{(1+t^2)^{\beta}} dy \right| \\
&\le \frac{2\beta \sin \pi\alpha}{\pi} \int_{-\infty}^{x} e^{t-x} \frac{|\psi(t)|}{(1+t^2)^{\beta}} dt \\
&\quad \times \left| (1+x^2)^{\beta} - \alpha \int_0^1 s^{\alpha-1} \big(1+(t+(x-t)s)^2\big)^{\beta} ds \right| \\
&\le \frac{2\beta \sin \pi\alpha}{\pi} \int_{-\infty}^{x} e^{t-x} \frac{|\psi(t)|}{(1+t^2)^{\beta}} \Big| (1+x^2)^{\beta} - (1+\min\{x^2,t^2\})^{\beta} \Big| dt \\
&\le \frac{2\beta \sin \pi\alpha}{\pi} \int_{-\infty}^{x} e^{t-x} \frac{|\psi(t)|}{(1+t^2)^{\beta}} \Big| (1+x^2)^{\beta} - (1+t^2)^{\beta} \Big| dt
\end{aligned}$$

$$\leq \frac{2\beta\sin\pi\alpha}{\pi}\int_{-\infty}^{x} e^{t-x}(1+(x-t)^2)^{\beta}\frac{|\psi(t)|}{(1+t^2)^{\beta}}dt$$
$$= \frac{2\beta\sin\pi\alpha}{\pi}e^{-x}(1+x^2)^{\beta}h(x) * \frac{|\psi(x)|}{(1+x^2)^{\beta}},$$

where $*$ denotes the Fourier convolution and $h(x) = \frac{1+\mathrm{sgn}(x)}{2}$ is the Heaviside function. Since $\kappa_\beta = \|e^{-x}h(x)(1+x^2)^{\beta}\|_{L^1(\mathbb{R})} = \int_0^\infty e^{-x}(1+x^2)^{\beta}dx < \infty$, the theorem of Young ([2, p.90]) implies $\|\mathcal{K}\psi\|_{L^2(\mathbb{R})} \leq \frac{2\beta\kappa_\beta\sin\pi\alpha}{\pi}\|\psi\|_{L^2(\mathbb{R})}$.

Second, taking into account $J_+^{\alpha,1}\phi = \frac{e^{-x}h(x)x^{\alpha-1}}{\Gamma(\alpha)} * \phi$ and the formula [12, p.163]

$$\frac{\pi}{\sin\pi\alpha}\frac{1}{b-x}\left|\frac{x-a}{x-b}\right|^{\alpha-1} = \int_a^b \frac{(y-a)^{\alpha-1}(b-y)^{-\alpha}}{y-x}dy, \quad x<a \text{ or } x>b,$$

we arrive at the identity $J_+^{\alpha,1}[(1+x^2)^{-\beta}\psi] = (1+x^2)^{-\beta}J_+^{\alpha,1}[\psi+\mathcal{K}\psi]$, which yields (13) with $c_{\alpha,\beta} = 1 + (2\beta\kappa_\beta\sin\pi\alpha)/\pi$. □

Corollary 1. *Let $f \in L^2(\mathbb{R})$ and $\alpha, \beta > 0$, then*

$$\big\|(1+x^2)^{\beta}J_\pm^{-\alpha,1}f\big\|_{L^2(\mathbb{R})} \leq c_{2\beta,\alpha/2}\big\|J_\pm^{-\alpha,1}[(1+x^2)^{\beta}f]\big\|_{L^2(\mathbb{R})}, \tag{14}$$

where $c_{\alpha,\beta} > 0$ is the same as in Lemma 1.

Proof. By (12),

$$\big\|(1+x^2)^{\beta}J_\pm^{-\alpha,1}f\big\|_{L^2(\mathbb{R})} = \big\|J_\pm^{-\beta,1}J_\mp^{-\beta,1}[(1+s^2)^{\alpha/2}\tilde{f}]\big\|_{L^2(\mathbb{R})}$$

and

$$\big\|J_\pm^{-\alpha,1}[(1+x^2)^{\beta}f]\big\|_{L^2(\mathbb{R})} = \big\|(1+s^2)^{\alpha/2}J_\pm^{-\beta,1}J_\mp^{-\beta,1}\hat{f}\big\|_{L^2(\mathbb{R})},$$

where $\hat{f} = \mathcal{F}[f]$ and $\tilde{f} = \frac{(1\mp is)^{\alpha/2}}{(1\pm is)^{\alpha/2}}\hat{f}$. Lemma 1 yields the result. □

In view of (10), (12), Lemma 1 and Corollary 1 it is convenient to work with the space

$$H^2_{\alpha,\beta}(\mathbb{R}) = \{f \mid \big\|J^{-\alpha,1}[(1+x^2)^{\beta/2}f]\big\|_{L^2(\mathbb{R})} < \infty\},$$

where $J^{-\alpha,1} = J_\pm^{-\alpha/2,1}J_\mp^{-\alpha/2,1}$. $H^2_{\alpha,\beta}(\mathbb{R})$ is a Hilbert space with respect to one of two inner products

$$\langle f,g\rangle_{H^2_{\alpha,\beta}(\mathbb{R})} = \int_{\mathbb{R}}(1+x^2)^{\beta}\Big(J^{-\alpha,1}[f]\Big)\Big(J^{-\alpha,1}[g]\Big)dx,$$
$$\langle f,g\rangle_{*,H^2_{\alpha,\beta}(\mathbb{R})} = \int_{\mathbb{R}}\Big(J^{-\alpha,1}[(1+x^2)^{\beta/2}f]\Big)\Big(J^{-\alpha,1}[(1+x^2)^{\beta/2}g]\Big)dx,$$

where the corresponding induced norms $\|\cdot\|_{H^2_{\alpha,\beta}(\mathbb{R})}$ and $\|\cdot\|_{*,H^2_{\alpha,\beta}(\mathbb{R})}$ are equivalent. We mention that $\mathcal{F}[H^2_{\alpha,\beta}(\mathbb{R})] = H^2_{\beta,\alpha}(\mathbb{R})$, i.e. $H^2_{\alpha,\beta}(\mathbb{R})$ is invariant under the Fourier transform. Note that $H^2_{\alpha,0}(\mathbb{R}) = H^{2,\alpha}(\mathbb{R})$ is a well known fractional order Sobolev space, see [2].

2.2.2. Approximation in $L^2(\mathbb{R})$

Let N be a positive integer, P_N a subspace of $L^2(\mathbb{R})$ spanned by $\{\phi_n\}_{n=0}^N$, $\hat{P}_N$ a subspace of $L^2(\mathbb{R})$ spanned by $\{\hat{\phi}_n\}_{n=0}^N$ and let $\mathcal{P}_N : L^2(\mathbb{R}^n) \to P_N$, $\hat{\mathcal{P}}_N : L^2(\mathbb{R}^n) \to \hat{P}_N$ denote the orthogonal projectors onto P_n and $\hat{P}_n$, respectively. Our task is to estimate $\|f - \mathcal{P}_N f\|_{L^2(\mathbb{R})} = \|\hat{f} - \hat{\mathcal{P}}_N f\|_{L^2(\mathbb{R})}$. We begin with a technical lemma.

Lemma 2. *Let $L_n^{(\alpha)}(s)$ be the generalized Laguerre polynomial of degree n and $Y_0(s)$ the Bessel function of the second kind (see [1]), then*

$$\hat{\phi}_0(s) = \frac{\sqrt{\pi\ell}}{2\sqrt{2}}\Big[Y_0(i\ell s) + Y_0(-i\ell s)\Big], \tag{15a}$$

$$\hat{\phi}_{2n}(s) = -\frac{\sqrt{\pi\ell}}{\sqrt{2}}\Big(J^{1,1}\frac{d}{ds}\mathrm{sgn}(s) + 1\Big)\Big[e^{-\ell|s|}L_n(2\ell|s|)\Big], \quad n \geq 1, \tag{15b}$$

$$\hat{\phi}_{2n+1}(s) = -i\frac{\sqrt{\pi\ell}}{\sqrt{2}}\mathrm{sgn}(s)e^{-\ell|s|}L_n(2\ell|s|), \quad n \geq 0. \tag{15c}$$

Proof. Formula (15a) is trivial. To establish (15b) and (15c) consider the generating functions

$$g_e(x,\xi) = \sum_{n\geq 0}\xi^n\phi_{2(n+1)} = \sqrt{\ell}\frac{(1-\xi)x^2 - (1+\xi)\ell^2}{(1-\xi)^2x^2 + (1+\xi)^2\ell^2},$$

$$g_o(x,\xi) = \sum_{n\geq 0}\xi^n\phi_{2n+1} = \frac{\sqrt{\ell}(1-\xi)x}{(1-\xi)^2x^2 + (1+\xi)^2\ell^2},$$

where $|\xi| < 1$. Their Fourier transforms are

$$\hat{g}_e(s,\xi) = -\frac{\sqrt{\pi\ell}}{\sqrt{2}}\Big(J^{1,1}\frac{d}{ds}\mathrm{sgn}(s) + 1\Big)\Big[\frac{1}{1-\xi}\exp\Big\{\frac{\xi 2\ell|s|}{\xi - 1}\Big\}\Big],$$

$$\hat{g}_o(s,\xi) = -i\frac{\sqrt{\pi\ell}}{\sqrt{2}}\mathrm{sgn}(s)e^{-\ell|s|}\frac{1}{1-\xi}\exp\Big\{\frac{\xi 2\ell|s|}{\xi - 1}\Big\},$$

since $\dfrac{\exp\{\xi s/(\xi - 1)\}}{(1-\xi)^{-\alpha-1}} = \sum\limits_{n\geq 0} L_n^{(\alpha)}(s)$, see [1, p. 784], the result follows. $\square$

It is convenient to study odd functions first.

Lemma 3. *Let $f \in H^2_{\alpha,\beta}$ be an odd function, then*

$$\|f - \mathcal{P}_N f\|_{L^2(\mathbb{R})} \leq \frac{c}{\min\{1, \ell^\gamma\}N^{\gamma/2}}\|f\|_{H^2_{\alpha,\beta}(\mathbb{R})}, \tag{16}$$

where γ=$\min\{2\alpha, \beta\}$. The positive constant c does not depend on N and f.

Proof. The assumptions of Lemma 3 imply that $\hat{f} \in H^2_{\beta,\alpha}$ and $\hat{f}$ is odd. Hence, the derivative $J_-^{-\gamma,\ell}\hat{f}(s)$ is well defined. Taking into account the definitions of Bessel fractional integroderivatives, formulas (11), (15c) and the identity [11, p. 462, formula 2.19.2.2]

$$J_+^{\gamma,\ell}[e^{-\ell s}L_n(2\ell s)h(s)] = \frac{\Gamma(n+1)}{\Gamma(n+\gamma+1)}s^\gamma e^{-\ell s}L_n^{(\gamma)}(2\ell s)h(s), \quad \Re\gamma > 0,$$

we obtain

$$\begin{aligned} a_{2n+1} &= \langle f, \phi_{2n+1}\rangle = \langle \hat{f}, \hat{\phi}_{2n+1}\rangle = -i\sqrt{2\pi\ell}\int_{\mathbb{R}} e^{-\ell s}L_n(2\ell s)h(s)\hat{f}(s)ds \\ &= -i\sqrt{2\pi\ell}\int_{\mathbb{R}} J_+^{-\gamma,\ell}J_+^{\gamma,\ell}[e^{-\ell s}L_n(2\ell s)h(s)]\hat{f}(s)ds \\ &= -i\sqrt{2\pi\ell}\int_{\mathbb{R}} J_+^{\gamma,\ell}[e^{-\ell s}L_n(2\ell s)h(s)]J_-^{-\gamma,\ell}[\hat{f}(s)]ds \\ &= -i\sqrt{2\pi\ell}\frac{\Gamma(n+1)}{\Gamma(n+\gamma+1)}\int_{\mathbb{R}} s^\gamma e^{-\ell s}L_n^{(\gamma)}(2\ell s)\Big(h(s)J_-^{-\gamma,\ell}[\hat{f}(s)]\Big)ds. \end{aligned}$$

The family $\{s^{\gamma/2}e^{-s/2}L_n^{(\gamma)}(s)\}_{n\geq 0}$ forms an orthogonal basis in $L^2(\mathbb{R}_+)$ [13, p. 108] and since $\|s^{\gamma/2}e^{-s/2}L_n^{(\gamma)}(s)\|^2_{L^2(\mathbb{R}_+)} = \dfrac{\Gamma(n+\gamma+1)}{\Gamma(n+1)}$, we have

$$\begin{aligned} \|f - \mathcal{P}_N f\|^2_{L^2(\mathbb{R})} &= \frac{2}{\pi}\sum_{n\geq[N/2]} a^2_{2n+1} \\ &= 4\ell\sum_{n\geq[N/2]}\frac{\Gamma^2(n+1)}{\Gamma^2(n+\gamma+1)}\left(\int_{\mathbb{R}} s^\gamma e^{-\ell s}L_n^{(\gamma)}(2\ell s)\Big(h(s)J_-^{-\gamma,\ell}[\hat{f}(s)]\Big)ds\right)^2 \\ &\leq \frac{2\Gamma([N/2]+1)}{(2\ell)^\gamma\Gamma([N/2]+\gamma+1)}\sum_{n\geq 0}\frac{(2\ell)^{\gamma+1}\Gamma(n+1)}{\Gamma(n+\gamma+1)} \\ &\quad \times\left(\int_{\mathbb{R}} s^{\gamma/2}e^{-\ell s}L_n^{(\gamma)}(2\ell s)\Big(s^{\gamma/2}h(s)J_-^{-\gamma,\ell}[\hat{f}(s)]\Big)ds\right)^2 \\ &= \frac{2\Gamma([N/2]+1)}{(2\ell)^\gamma\Gamma([N/2]+\gamma+1)}\Big\|s^{\gamma/2}J_-^{-\gamma,\ell}[\hat{f}(s)]\Big\|^2_{L^2(\mathbb{R}_+)}. \end{aligned}$$

Due to Lemma 1 and formula (12)

$$\frac{1}{\ell^\gamma}\Big\|s^{\gamma/2}J_-^{-\gamma,\ell}[\hat{f}(s)]\Big\|_{L^2(\mathbb{R}_+)} \leq \frac{c_{\gamma/2,\gamma}}{\min\{1,\ell^\gamma\}}\|f\|_{H^2_{\gamma/2,\gamma}(\mathbb{R})},$$

thus, estimate (16) is the consequence of Stirling's formula. □

For even functions we have a similar result.

Lemma 4. *Let $f \in H^2_{\alpha,\beta}$ be an even function, then*

$$\|f - \mathcal{P}_N f\|_{L^2(\mathbb{R})} \leq \frac{c}{\min\{1,\ell^\gamma\}N^{\gamma/2}}\|f\|_{H^2_{\alpha,\beta}(\mathbb{R})}, \tag{17}$$

where γ=min$\{2\alpha,\beta\}$. The positive constant c does not depend on N and f.

Proof. The proof is completely identical to that of Lemma 3 and it is omitted. □

Estimates (16) and (17) together yield

Theorem 1. *Let $f \in L^2_{\alpha,\beta}$, $\alpha, \beta \geq 0$ and $\gamma = \min\{2\alpha, \beta\}$, then*

$$\|f - \mathcal{P}_N f\|_{L^2(\mathbb{R})} \leq \frac{c}{\min\{1, \ell^\gamma\} N^{\gamma/2}} \|f\|_{H^2_{\alpha,\beta}(\mathbb{R})}, \tag{18}$$

where $c > 0$ does not depend on N and f.

We mention that inequality (16) improves the result of [9], where an estimate for Laguerre type spectral approximations is obtained using an interpolation of Sobolev spaces.

2.2.3. Pseudospectral discretization in space

Using the pseudospectral approach we shall replace u_k in (5) with its truncated spectral expansion. According to (6), the spectral coefficients are given by

$$u_{k,n} = \langle u_k, \phi_n \rangle = \int_{\mathbb{R}} (u_k(x), \phi_n(x)) dx = \int_0^\pi \frac{u_k(\xi)}{\sin \xi} \cos n\xi d\xi, \quad 0 \leq n \leq N-1,$$

where $\xi = \operatorname{arccot} \dfrac{x}{\ell}$. In practice, the coefficient $u_{k,n}$ cannot be computed exactly and the integral must be replaced with a quadrature formula. Since $u_k \in L^2(\mathbb{R})$, i.e. $u(\pm\infty) = 0$, we use Gauss quadrature

$$\tilde{u}_{k,j} = \frac{2}{N} \sum_{n=0}^{N-1} \frac{u_k(\xi_n)}{\sin(\xi_n)} \cos j\xi_n, \quad \xi_n = \frac{2n+1}{2N}\pi, \tag{19}$$

$0 \leq n \leq N-1, \quad 0 \leq j \leq N-1.$

It is straightforward to verify that the discrete expansion interpolates $u_k(x)$ at the Gaussian points, i.e.

$$\tilde{u}_k(x_n) = \frac{\tilde{u}_{k,0}}{\pi} \phi_0(x_n) + \sum_{j=1}^{N-1} \frac{2\tilde{u}_{k,j}}{\pi} \phi_j(x_n), \quad x_n = \ell \cot \frac{2n+1}{2N}\pi. \tag{20}$$

$0 \leq n \leq N-1.$

Thus, we can write $\tilde{u}_k = \mathcal{I}_N u_k$, where $\mathcal{I}_N$ is the interpolation operator defined by (19) and (20). The simplest space discretization of (5) is obtained if we replace the quantities u, $e^{\mathcal{L}} u$ and $\psi(\mathcal{L}) f(u)$ with their interpolants $\mathcal{I}_N u$, $\mathcal{I}_N e^{\mathcal{L}} \tilde{u}$ and $\mathcal{I}_N \psi(\mathcal{L}) \mathcal{I}_N f(\tilde{u})$, respectively.

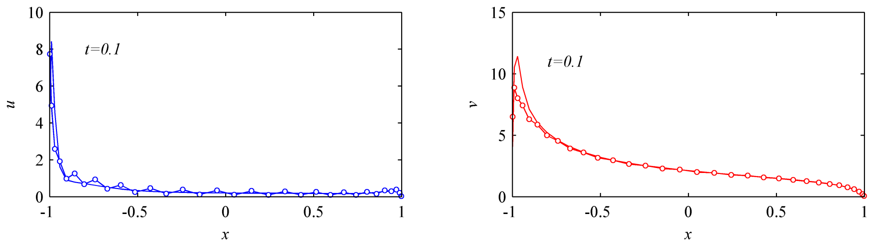

Figure 1.

The resulting numerical scheme is explicit both in time and space. Its local order of approximation is four in time. Order of approximation in space is given by Theorem 1. Unfortunately, numerical experiments show that the method is numerically unstable. The problem is that the nonlinear terms $\mathcal{I}_N f(\tilde{u})$ rapidly amplify the approximation error introduced by the truncated discrete expansion of u_k. As a result, after a short time the numerical solution develops parasitic high frequency spatial oscillations and the numerical scheme blows up. The standard solution to the problem is to use filtering, see [4, 5, 6]. In our computations we use the simplest second order filter (the raised cosine filter)

$$\mathcal{F}_N u = \frac{1}{\pi} \sum_{j=0}^{N-1} \tilde{u}_j \left(1 + \cos\Big(\frac{j}{N}\Big)\right) \phi_j.$$

The resulting method takes the form

$$\begin{aligned}
\tilde{u}_{k,1} &= \mathcal{I}_N \Big(e^{\frac{\tau}{2}\mathcal{L}} \tilde{u}_k + \frac{\tau}{2} \psi_{1,2}(\tau\mathcal{L}) \mathcal{F}_N f(\tilde{u}_k) \Big), && \text{(21a)}\\
\tilde{u}_{k,2} &= \mathcal{I}_N \Big(e^{\frac{\tau}{2}\mathcal{L}} \tilde{u}_k + \tau \Big[\frac{1}{2}\psi_{1,2} - \psi_{2,2}\Big](\tau\mathcal{L}) \mathcal{F}_N f(\tilde{u}_k) && \text{(21b)}\\
&\quad + \tau \psi_{2,2}(\tau\mathcal{L}) \mathcal{F}_N f(\tilde{u}_{k,1}) \Big),\\
\tilde{u}_{k,3} &= \mathcal{I}_N \Big(e^{\tau\mathcal{L}} \tilde{u}_k + \tau \Big[\psi_1 - 2\psi_2\Big](\tau\mathcal{L}) \mathcal{F}_N f(\tilde{u}_k) && \text{(21c)}\\
&\quad + \tau \psi_2(\tau\mathcal{L}) \mathcal{F}_N \Big[f(\tilde{u}_{k,1}) + f(\tilde{u}_{k,2}) \Big] \Big),\\
\tilde{u}_{k,4} &= \mathcal{I}_N \Big(e^{\frac{\tau}{2}\mathcal{L}} \tilde{u}_k + \tau \Big[\frac{1}{2}\psi_{1,2} - 2a_{5,2} - a_{5,4}\Big](\tau\mathcal{L}) \mathcal{F}_N f(\tilde{u}_k) && \text{(21d)}\\
&\quad + \tau a_{5,2}(\tau\mathcal{L}) \mathcal{F}_N \Big[f(\tilde{u}_{k,1}) + f(\tilde{u}_{k,2}) \Big] + \tau a_{5,4}(\tau\mathcal{L}) \mathcal{F}_N f(\tilde{u}_{k,3}) \Big),\\
\tilde{u}_{k+1} &= \mathcal{I}_N \Big(e^{\tau\mathcal{L}} \tilde{u}_k + \tau \Big[\psi_1 - 3\psi_2 + 4\psi_3\Big](\tau\mathcal{L}) \mathcal{F}_N f(\tilde{u}_k) && \text{(21e)}\\
&\quad + \tau \Big[4\psi_3 - \psi_2\Big](\tau\mathcal{L}) \mathcal{F}_N f(\tilde{u}_{k,3}) + \tau \Big[4\psi_2 - \psi_3\Big](\tau\mathcal{L}) \mathcal{F}_N f(\tilde{u}_{k,4}) \Big).
\end{aligned}$$

The filter efficiently damps all parasitic spatial oscillations and the resulting method is stable and suitable for long time numerical simulations. The smoothing effect of $\mathcal{F}_N$ is illustrated in Fig. 1.

3. Computational aspects

Method (21) requires five discrete expansions of the form $\mathcal{I}_N f(u)$ and twenty "function of operator-vector products" of the form $\psi(\tau\mathcal{L})u$ per time step. Here we discuss how to organize these computations efficiently.

3.1. Fast spectral transform

The discrete expansions (19) can be efficiently calculated via the standard discrete fast Fourier transform (FFT). For this we set

$$v_n = e^{-i\frac{2\pi n}{N}} \begin{cases} u_k(\xi_{2n}), & 0 \le n \le \frac{N}{2} - 1; \\ -u_k(\xi_{2N-2n-1}), & \frac{N}{2} \le n \le N-1; \end{cases} \tag{22a}$$

and apply FFT to the sequence v_n

$$\tilde{v}_j = \sum_{n=0}^{N-1} v_n e^{-i\frac{2\pi j n}{N}}, \quad 0 \le j \le N-1. \tag{22b}$$

The coefficients $\tilde{u}_{k,j}$ are obtained by means of the formula

$$\tilde{u}_{k,j} = \tilde{u}_{k,j+2} + \frac{2i}{N}\Big(e^{-i\frac{\pi(j+1)}{2N}}\tilde{v}_j - e^{i\frac{\pi(j+1)}{2N}}\tilde{v}_{N-j-2}\Big), \quad 0 \le j \le N-2, \tag{22c}$$

$$\tilde{u}_{k,N-1} = \tfrac{2}{N}\tilde{v}_{N-1}, \qquad \tilde{u}_{k,N} = 0. \tag{22d}$$

Note that (22) avoids explicit evaluations of the fractions $\dfrac{u_k(\xi_n)}{\sin\xi_n}$ which are not well defined numerically when abscissas ξ_n are close to the boundary points 0 and π. Fast inverse transform (20) is obtained by inverting (22).

3.2. Evaluation of "function of operator times vector"

At each time step we have to approximate few expressions of the form $\psi(\tau\mathcal{L})u$, where $u \in \operatorname{span}\{\phi_j | 0 \le j \le N-1\}$. This can be efficiently done by means of the Krylov subspace method, see [7]. The identity

$$\begin{aligned} -\triangle\phi_j =& \frac{1}{16}\Big((j-1)(j-3)\phi_{|j-4|} - 4(j-1)^2\phi_{|j-2|} \\ &+ (6j^2+2)\phi_j - 4(j+1)^2\phi_{j+2} + (j+1)(j+3)\phi_{j+4}\Big) \end{aligned}$$

shows that in the mode space the Laplacian is represented by infinite dimensional five diagonal matrix and the action $\mathcal{L}u$ is easily evaluated. Applying the Arnoldi process to $\mathcal{L}$ we obtain an orthonormal basis $U_m = [u_1, \ldots, u_m]$ of the Krylov subspace $K_m = \operatorname{span}\{\mathcal{L}^j u | 0 \le j \le m-1\}$ and the upper Hessenberg matrix $H_m \in \mathbb{R}^{m\times m}$ such that

$$\mathcal{L}U_m = H_m U_m + h_{m+1,m} u_{m+1} e_m^T,$$

where e_m is the m-th unit vector. The approximation is given by

$$\psi(\tau\mathcal{L})u \approx U_m \psi(\tau H_m) e_1, \quad m \ge 1. \tag{23}$$

The analysis of (23) in finite dimensional settings can be found in [7]. Its modification to infinite dimensions is straightforward. The convergence rate of (23) is normally very fast, in our case the algorithm requires from 3 to 7 iterations to approximate $\psi(\tau\mathcal{L})u$ with the accuracy of 10^{-5}.

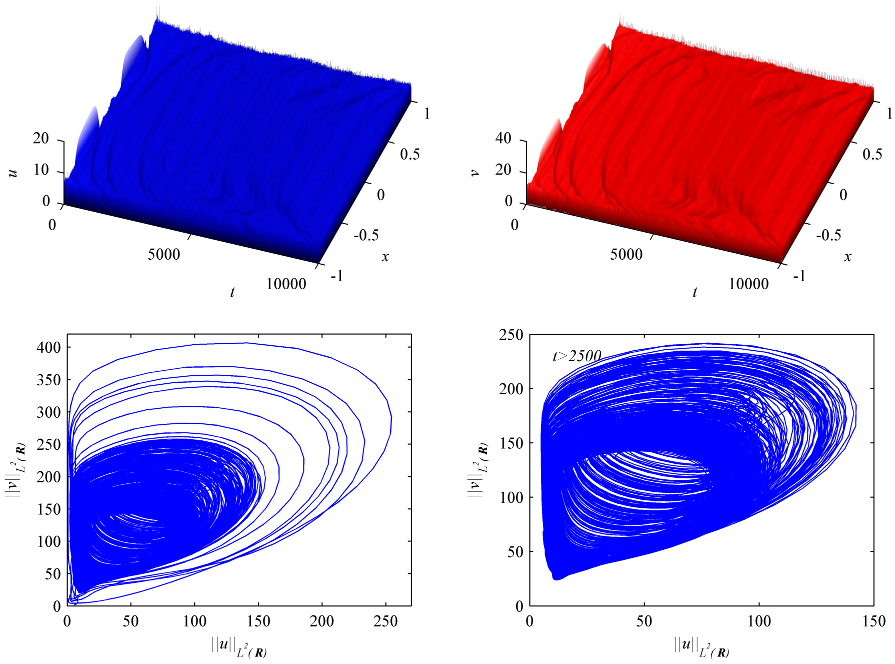

Figure 2. *Numerical solution of (1) with* $a_1 = 10^{-5}$, $a_2 = 10^{-6}$ *and initial conditions (24)*

4. Numerical simulation

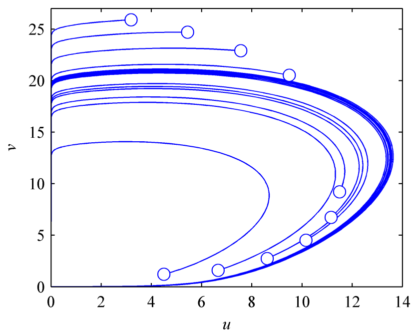

Figure 3.

For numerical simulations we set $A = \frac{1}{5}$, $K = 100$, and $a = k = c = g = B = 1$. With this choice of the parameters the ordinary differential equation (equation (1) with $a_1 = a_2 = 0$) has a limit cycle, see Fig. 1. In our first experiment we set

$N = 1024$, $a_1 = 10^{-5}$, $a_2 = 10^{-6}$,

$$u_0(x) = \frac{10e^{-10\cos^8\left(\pi x/\sqrt{1+x^2}\right)}}{\sqrt{1+x^2}}, \tag{24a}$$

$$v_0(x) = \frac{2}{\sqrt{1+x^2}} + \frac{x}{(1+x^2)^2}, \tag{24b}$$

and integrate (1) using (21) in the interval $[0, 10^4]$. Solutions are shown in the two upper diagrams of Fig. 2. The dynamics of both components u and v are very

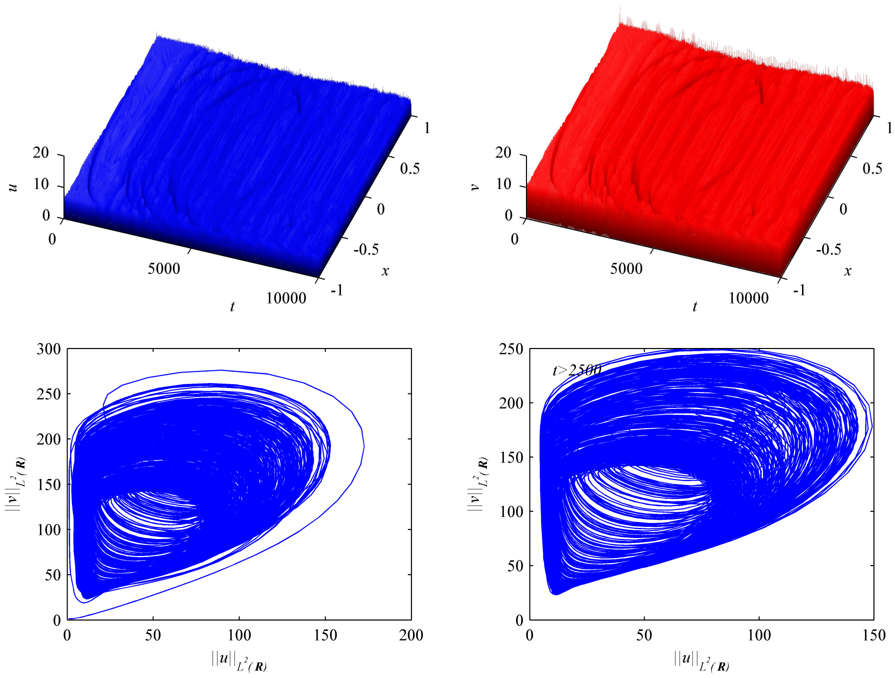

Figure 4. *Numerical solution of (1) with* $a_1 = 10^{-5}$, $a_2 = 10^{-6}$ *and initial conditions (25), (24b)*

complicated. One can observe that from time to time the trajectories split into a large number of irregular patches which slowly travel towards the boundaries. A more descriptive account on the behavior of (1) is provided by the two lower diagrams of Fig. 2. The left plot shows the phase portrait of the spatial averages $\|u(t)\|_{L^2(\mathbb{R})}$ and $\|v(t)\|_{L^2(\mathbb{R})}$. The phase trajectory is bounded and almost entirely fills some region in the phase space. The structure of the region is seen better in the right diagram where the phase trajectory for $t \in [2500, 10^4]$ is plotted. It is important to mention that in the last diagram the trajectory is separated away from the coordinate axes (compare to Fig. 3), thus, the presence of a small diffusion in the model (1) ensures the coexistence of the species.

In the second experiment we repeat our previous simulation with

$$u_0(x) = \frac{1}{\sqrt{1+x^2}} - \frac{x^3}{(1+x^2)^2} \tag{25}$$

and (24b). The results are qualitatively the same as before (compare two lower diagrams in Fig. 2 and Fig. 4). We tested (1) using various initial data, in all these runs the long time behavior remains the same as in Figs. 2 and 4. This agrees with the results of [14] where the existence of a global attractor is established.

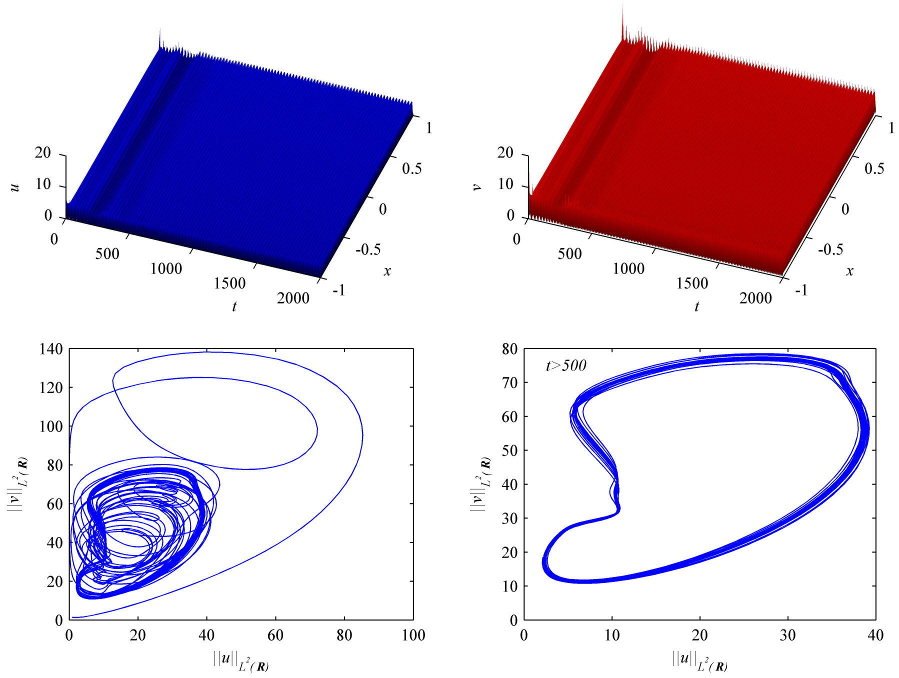

Figure 5. *Numerical solution of (1) with* $a_1 = a_2 = 1$ *and initial conditions (25), (24b)*

For our final test run we set $N = 256$, $a_1 = a_2 = 1$ and use the initial conditions (25) and (24b). With these settings the dynamics of (1) is relatively simple. After a short period of time the large diffusion coefficients almost equidistribute u and v over the spatial domain (see two upper diagrams in Fig. 5). The phase portraits of the averaged densities are provided in the lower diagrams of Fig. 5. Once again there is a noticeable gap between the phase trajectory and the axes when $t > 500$, hence, both species do coexist.

To conclude this section we emphasize that the ecological model (1) based on the ODE ($a_1 = a_2 = 0$) leads to a pessimistic scenario where both ecological species are practically extinct (see Fig. 3). Nonetheless, the numerical simulations indicate that in the presence of (even tiny) diffusion the species may safely coexist. Hence, the spatial interaction between the species cannot be eliminated in the present ecological model.

Concluding remarks

In the present paper we proposed an efficient algorithm for simulating a reaction-diffusion equation posed in the entire space $\mathbb{R}^d$. The numerical algorithm is applied to a practical model taken from mathematical ecology. However, the method is sufficiently general to be used in other areas of applied sciences.

The analysis of the spatial discretization error based on the use of Bessel fractional integroderivatives leads to sharper error bounds in $L^2(\mathbb{R})$, as compared to previously known results. The extension of this approach to general Sobolev spaces is currently under investigation.

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