Numerical solutions of the variable-order space fractional activator-inhibitor reaction-diffusion systems

Redouane Douaifia[a], Salem Abdelmalek[a,b]

[a] *Laboratory of Mathematics, Informatics and Systems (LAMIS), Larbi Tebessi University – Tebessa, Algeria*
[b] *Department of Mathematics and Computer Science, Larbi Tebessi University – Tebessa, Algeria*

Abstract

Reaction–diffusion equations containing fractional derivatives can provide adequate mathematical models for explaining anomalous diffusion and transport dynamics in complex systems that can not be adequately modeled by standard numerical order equations. Researchers have recently found that many physical processes display fractional order dynamics that differs with time or space. The continuity of order in the fractional calculation allows the order of the fractional operator to be regarded as a variable. The Samko–Ross variable-order fractional operator can be viewed as a generalization of the Riemann–Liouvile type definition. Although this definition is the most appropriate definition having fundamental characteristics that are desirable for physical modeling, numerical methods for reaction–diffusion activator–inhibitor systems using this definition have not yet appeared in the literature. In this paper, we provide a numerical method to get the approximate solutions of the variable-order space-fractional Activator–inhibitor systems, namely the reaction–diffusion system with cubic nonlinearity and Brusselator model on a 1–D space–domain, we adopt the Riesz variable–order space fractional derivative. Numerical simulations demonstrate that the finite difference approach is computationally efficient.

Keywords

Variable–order calculus, activator–inhibitor systems, numerical simulation

1. Introduction

In recent decades, fractional derivatives have been commonly used in the modeling of complex physical and mechanical phenomena in wide classes of complex media with hereditary, fractal and non-markovian properties, is a field of rapidly growing interest with applications in many different fields. These include the study of biology [1], hydrology [2], biochemistry [3], finance [4], and physics [5]. But researchers have found that many important dynamic processes show fractional order behavior that may change with time and / or space. This fact suggests that differential calculus is a natural candidate to provide an effective mathematical framework to describe the complex dynamic problems that appear in different biological and chemical models, such as viscoelastic materials, anomalous diffusion. In reaction diffusion systems which can be described by two variables, one has the notion of an activator and an inhibitor. In that case, be the diffusion coefficient of the inhibitor greater than the diffusion coefficient of the

IAM'20: Third conference on informatics and applied mathematics, 21–22 October 2020, Guelma, ALGERIA
redouane.douaifia@univ–tebessa.dz (R. Douaifia); salem.abdelmalek@univ–tebessa.dz (S. Abdelmalek)
0000-0001-6960-4572 (R. Douaifia); 0000-0001-9762-9654 (S. Abdelmalek)

activator if spontaneous steady-state patterns are to occur. Thus, pattern formation is said to occur as a result of "short range activation" and "long range inhibition", the activator-inhibitor reaction-diffusion systems model was used to simulate pattern forming processes. In this work we show the behavior of solutions for activator-inhibitor models with variable superdiffusion by remplacing the second derivative in space by the variable order Riesz fractional derivative. The studies of dynamics and numerical simulations of fractional-space activator–inhibitor reaction–diffusion systems have recently met with the interest of researchers (cf. [6, 7]).

2. Variable–order fractional derivative

In [8, 9] Samko and Ross directly generalized the Riemann-Liouvile and Marchaud fractional integration and differentiation of the case of variable order and discussed some properties and the inversion formula . It has become a controversial research and has raised widespread concern in the last years.

This section is devoted to the most important definitions of variable–order direvatives.

2.1. Variable–order Riemann–Liouville fractional derivatives

Left derivative:

$$ {}_aD_x^{\alpha(t,x)}u(t,x) = \left[\frac{1}{\Gamma(m-\alpha(t,x))}\frac{\partial^m}{\partial\xi^m}\int_a^\xi(\xi-\lambda)^{m-\alpha(t,x)-1}u(t,\lambda)d\lambda\right]_{\xi=x}$$

Right derivative:

$$ {}_xD_b^{\alpha(t,x)}u(t,x) = \left[\frac{(-1)^m}{\Gamma(m-\alpha(t,x))}\frac{\partial^m}{\partial\xi^m}\int_\xi^b(\lambda-\xi)^{m-\alpha(t,x)-1}u(t,\lambda)d\lambda\right]_{\xi=x}$$

where $\Gamma(.)$ is gamma function and $m-1<\alpha(t,x)\leqslant m$, $m\in\mathbb{N}$.

2.2. Variable-order Grünwald-Letnikov fractional derivatives

Left derivative:

$$ {}_a^GD_x^{\alpha(t,x)}u(t,x) = \lim_{h\longrightarrow 0, nh=x-a} h^{-\alpha(t,x)}\sum_{j=0}^{n}(-1)^j\binom{\alpha(t,x)}{j}u(t,x-jh)$$

Right derivative:

$$ {}_x^GD_b^{\alpha(t,x)}u(t,x) = \lim_{h\longrightarrow 0, nh=b-x} h^{-\alpha(t,x)}\sum_{j=0}^{n}(-1)^j\binom{\alpha(t,x)}{j}u(t,x+jh)$$

where

$$\binom{\alpha(t,x)}{j} = \frac{\Gamma(\alpha(t,x)+1)}{\Gamma(j+1)\Gamma(\alpha(t,x)-j+1)},$$

and $m-1<\alpha(t,x)\leqslant m$, $m\in\mathbb{N}$.

2.3. Variable–order Riesz fractional derivative

$$\frac{\partial^{\alpha(t,x)}u(t,x)}{\partial |x|^{\alpha(t,x)}} = -\frac{1}{2\cos\left(\frac{\pi\alpha(t,x)}{2}\right)}\left[{}_aD_x^{\alpha(t,x)}u(t,x) +_x D_b^{\alpha(t,x)}u(t,x)\right].$$

3. General Activator-inhibitor model

Consider a 2-species reaction-diffusion system

$$\frac{\partial u}{\partial t} = D_u\Delta u + F(u,v), \qquad \frac{\partial v}{\partial t} = D_v\Delta v + G(u,v)$$

Assume there exists a constant steady state $E_{eq} = (u_{eq}, v_{eq})$,

$$F(u_{eq}, v_{eq}) = G(u_{eq}, v_{eq}) = 0$$

The Jacobian of the previous system is defined by

$$J|_{E_{eq}} = \begin{pmatrix} J_{11} & J_{12} \\ J_{21} & J_{22} \end{pmatrix} = \begin{pmatrix} \frac{\partial F}{\partial u}|_{E_{eq}} & \frac{\partial F}{\partial v}|_{E_{eq}} \\ \frac{\partial G}{\partial u}|_{E_{eq}} & \frac{\partial G}{\partial v}|_{E_{eq}} \end{pmatrix}$$

We say that the reaction diffusion system is the inhibitory activator system if the coefficients of its Jacobian matrix have the following relationships:

$$J_{11}J_{22} < 0, \qquad J_{12}J_{21} < 0$$

The species that achieve $J_{ii} > 0$, ($J_{ii} < 0$) is called activator (inhibitor), respectively ($i = 1, 2$).

4. The variable order space fractional Activator-inhibitor models

4.1. Variable order space fractional reaction–diffusion model with cubic nonlinearity

We consider the reaction-diffusion model with cubic nonlinearity in one-dimensional space, by replacing the classical spatial differential operators by variable order Riesz fractional analogues , we obtain the following system

$$\frac{\partial u}{\partial t} = D_u\frac{\partial^{\alpha(t,x)}u}{\partial |x|^{\alpha(t,x)}} + u - \frac{1}{3}u^3 - v, \qquad \text{in} \quad [0,T]\times[a,b], \tag{1}$$

$$\frac{\partial v}{\partial t} = D_v\frac{\partial^{\alpha(t,x)}v}{\partial |x|^{\alpha(t,x)}} + u - v + A, \qquad \text{in} \quad [0,T]\times[a,b], \tag{2}$$

and the initial and boundary conditions

$$u(0,x) = u_0(x), \quad v(0,x) = v_0(x), \quad \text{on} \quad [a,b], \tag{3}$$

$$u(t,a) = u(t,b) = BC_u, \qquad v(t,a) = v(t,b) = BC_v, \ \ \forall t \in [0,T]\,. \tag{4}$$

Here u, v represent the concentrations of two species having the diffusion rates $D_u, D_v > 0$, $A \in \mathbb{R}$, $BC_u \geqslant 0$ and $BC_v \geqslant 0$ are external parameters.

4.2. Variable order space fractional Brusselator model

We consider the well-known reaction-diffusion model Brusselator in one-dimensional space, by replacing the classical spatial differential operators by variable order Riesz fractional analogues , we get the following system

$$\frac{\partial u}{\partial t} = D_u \frac{\partial^{\alpha(t,x)} u}{\partial |x|^{\alpha(t,x)}} + A - (B+1)u + vu^2, \qquad \text{in} \quad [0,T] \times [a,b]\,, \tag{5}$$

$$\frac{\partial v}{\partial t} = D_v \frac{\partial^{\alpha(t,x)} v}{\partial |x|^{\alpha(t,x)}} + Bu - vu^2, \qquad \text{in} \quad [0,T] \times [a,b]\,, \tag{6}$$

and the initial and boundary conditions

$$u(0,x) = u_0(x), \ \ v(0,x) = v_0(x), \quad \text{on} \quad [a,b]\,, \tag{7}$$

$$u(t,a) = u(t,b) = BC_u, \qquad v(t,a) = v(t,b) = BC_v, \ \ \forall t \in [0,T]\,. \tag{8}$$

The species u, v represent the concentrations of two intermediary reactants having the diffusion rates $D_u, D_v > 0$ and $A, B > 0$ are fixed concentrations, and BC_u, BC_v are external parameters (nonnegative numbers).

5. Explicit Euler Approximation

We show the approximate solutions for systems (1)-(4) and (5)-(8) by applying the explicit finite difference method which described in [10].

We consider the numerical approximation in the time domain $[0,T]$ and the space domain $[a,b]$. Let $t_k = k\Delta t \ \ (0 \leqslant t_k \leqslant T)$, $k = 0, \dots, M$,

$x_i = a + i\Delta x \ \ (a \leqslant x_i \leqslant b)$, $i = 0, \dots, N$, where the time step is $\Delta t = \frac{T}{M}$ and the space step is $\Delta x = \frac{b-a}{N}$. We denote that $u_i^k = u(t_k, x_i)$, $\alpha_i^k = \alpha(t_k, x_i)$, $c_i^k = -\frac{\sec(\pi\alpha_i^k)}{2}$. The approximate Grünwald formulas for the variable-order Riemann-Liouville fractional derivatives approximation show as follow:

$${}_aD_{x_i}^{\alpha_i^k} u(t_k, x_i) = {}_a^G D_{x_i}^{\alpha_i^k} u(t_k, x_i) \approx (\Delta x)^{-\alpha_{i+1}^k} \sum_{j=0}^{i+1} g_{\alpha_{i+1}^k}^{(j)} u_{i+1-j}^k$$

$${}_{x_i}D_b^{\alpha_i^k} u(t_k, x_i) = {}_{x_i}^G D_b^{\alpha_i^k} u(t_k, x_i) \approx (\Delta x)^{-\alpha_{i-1}^k} \sum_{j=0}^{N-i+1} g_{\alpha_{i-1}^k}^{(j)} u_{i-1+j}^k$$

where $g_{\alpha_i^k}^{(j)}$ is the Grünwald weights defined by

$$g_{\alpha_i^k}^{(0)} = 1, \ \ g_{\alpha_i^k}^{(j)} = \left(1 - \frac{\alpha_i^k + 1}{j}\right) g_{\alpha_i^k}^{(j-1)}, \ \ (j = 1, 2, \dots)$$

Therefore, the equations (1)-(2) and (5)-(6) can be discretized as follow:

$$u_i^{k+1} = u_i^k + D_u \left(r_{i,k}^{(1)} \sum_{j=0}^{i+1} g_{i+1,k}^{(j)} u_{i+1-j}^k + r_{i,k}^{(2)} \sum_{j=0}^{N-i+1} g_{i-1,k}^{(j)} u_{i-1+j}^k \right) + \Delta t F(u_i^k, v_i^k) \tag{9}$$

$$v_i^{k+1} = v_i^k + D_v \left(r_{i,k}^{(1)} \sum_{j=0}^{i+1} g_{i+1,k}^{(j)} v_{i+1-j}^k + r_{i,k}^{(2)} \sum_{j=0}^{N-i+1} g_{i-1,k}^{(j)} v_{i-1+j}^k \right) + \Delta t G(u_i^k, v_i^k) \tag{10}$$

where $r_{i,k}^{(1)} = \Delta t c_i^k (\Delta x)^{-\alpha_{i+1}^k}$, $r_{i,k}^{(2)} = \Delta t c_i^k (\Delta x)^{-\alpha_{i-1}^k}$, $g_{i,k}^{(j)} = g_{\alpha_i^k}^{(j)}$ and

$$\begin{cases} F(u_i^k, v_i^k) &= u_i^k - \frac{1}{3}(u_i^k)^3 - v_i^k \\ G(u_i^k, v_i^k) &= u_i^k - v_i^k + A \end{cases} \quad or \quad \begin{cases} F(u_i^k, v_i^k) &= A - (B+1)u_i^k + v_i^k (u_i^k)^2 \\ G(u_i^k, v_i^k) &= Bu_i^k - v_i^k (u_i^k)^2 \end{cases}$$

The stability and convergence of the explicit Euler approximation are descused in [10].

6. Numerical experiments

In this section, we show approximate solutions for the systems (1)-(4) and (5)-(8) to demonstrate the changes in solutions behaviour that arise when the exponent is varied from integer order to fractional order to variable order, and to identify the differences between solutions. The computer algorithm for numerical method (9)-(10), was written in Matlab, throughout the simulations we took the following values: $a = 0$, $b = 4$, $T = 20$, spatial and time steps respectively $\Delta x = \frac{4}{20}$, $\Delta t = \frac{(\Delta x)^2}{2} - 0.001$.

6.1. Reaction-diffusion model with cubic nonlinearity

We take, $A = -0.1$, $D_u = 0.05$, $D_v = 1$, $BC_u = 0.0503$, $BC_v = 0.07504$ and the initial conditions:

$$\begin{cases} u_0(x) &= 0.0503 - 10^{-3}\cos(2\pi x) + 10^{-3}\cos(5\pi x) \\ v_0(x) &= 0.02504 + 10^{-3}\cos(2\pi x) + 10^{-3}\cos(5\pi x) \end{cases}$$

The figure 1 shows the approximate solution for system (1)-(4) for $\alpha(t,x) = 2$, when the derivative is fractional order $\alpha(t,x) = 1.35$ we can see the sulotions in figure 2. The behaviour of the solution is particularly interesting for the case $\alpha(t,x) = 1.5 + 0.4\cos(tx) * \sin(2t)$, see figure 3.

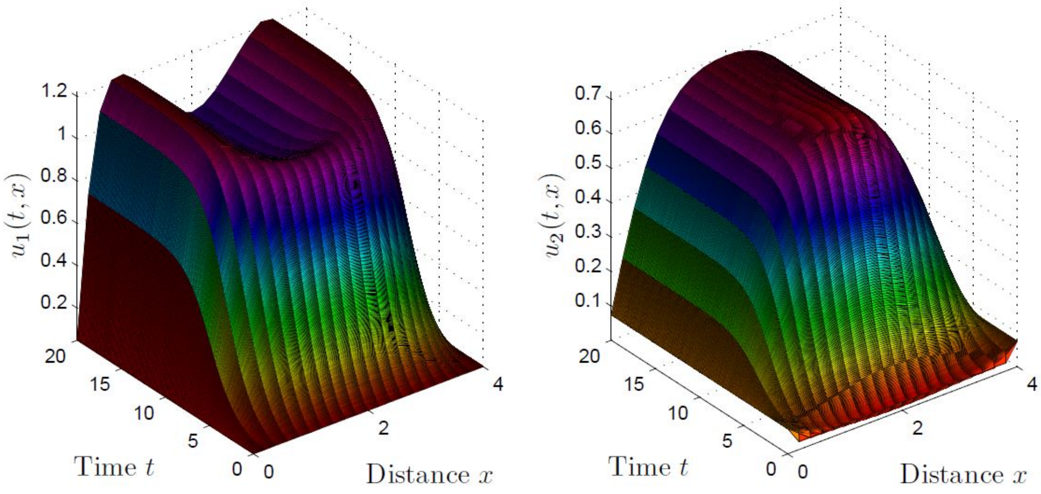

Figure 1: Approximate solution of (1)-(4), for $\alpha(t,x) = 2$, where $u_1 = u$ and $u_2 = v$.

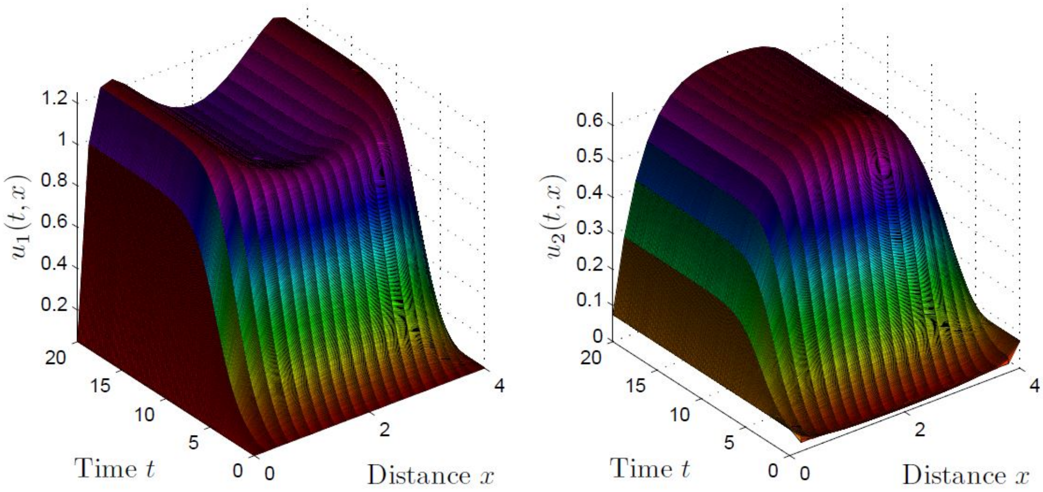

Figure 2: Approximate solution of (1)-(4), for $\alpha(t,x) = 1.35$, where $u_1 = u$ and $u_2 = v$.

6.2. Brusselator model

We take, $A = 1$, $B = 3$, $D_u = 0.05$, $D_v = 1$, $BC_u = 1.09$, $BC_v = 2.02504$ and the initial conditions:

$$\begin{cases} u_0(x) & = & 1.09 - 10^{-2}\cos(2\pi x) + 10^{-3}\cos(5\pi x) \\ v_0(x) & = & 2.02504 + 10^{-2}\cos(2\pi x) + 10^{-3}\cos(5\pi x) \end{cases}$$

Figure 4 shows the behavior of the numerical solution for system (5)-(8) with $\alpha(t,x) = 2$, when the derivative is fractional order $\alpha(t,x) = 1.35$ we can see the sulotions in figure 5. The

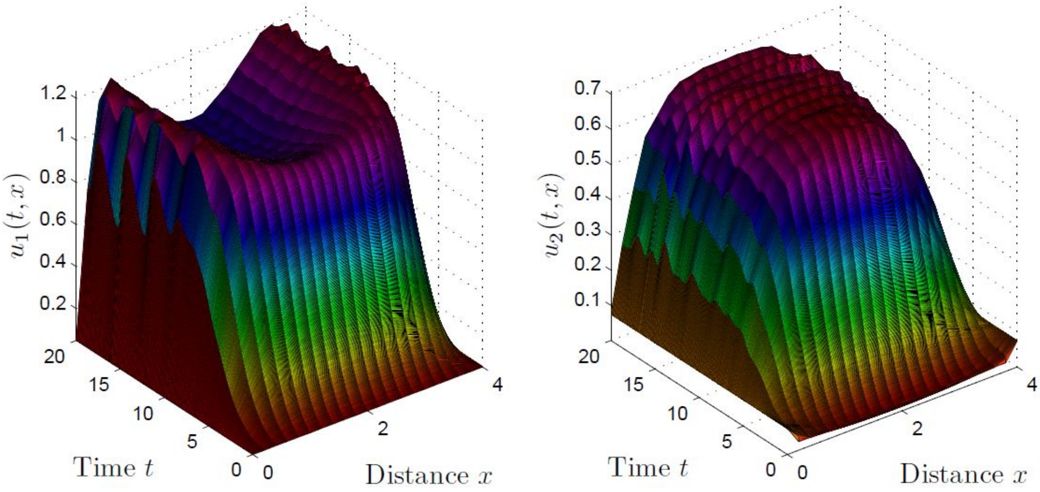

Figure 3: Approximate solution of (1)-(4), for $\alpha(t,x) = 1.5 + 0.4\cos(tx) * \sin(2t)$, where $u_1 = u$ and $u_2 = v$.

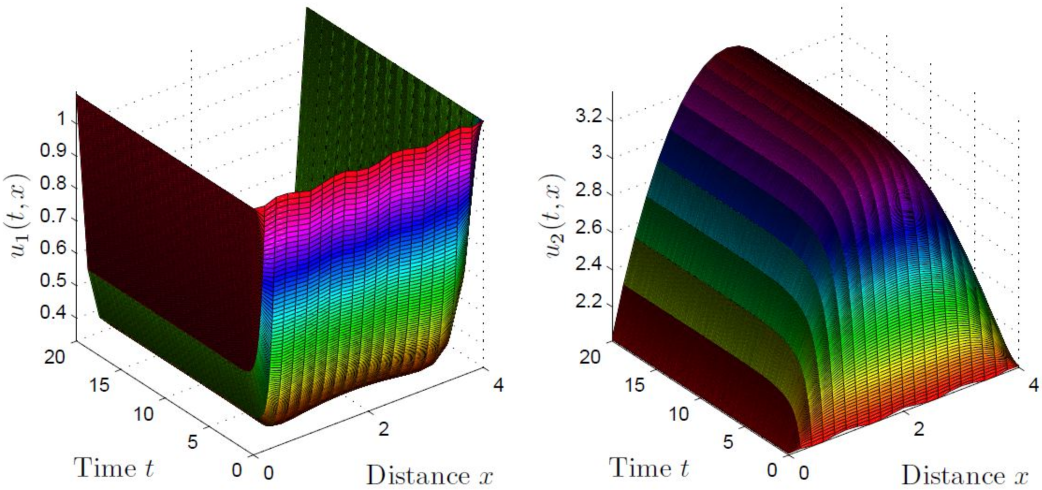

Figure 4: Approximate solution of (5)-(8), for $\alpha(t,x) = 2$, where $u_1 = u$ and $u_2 = v$.

behaviour of the solution is particularly interesting for the case $\alpha(t,x) = 1.5 + 0.4\cos(tx) * \sin(2t)$, see figure 6.

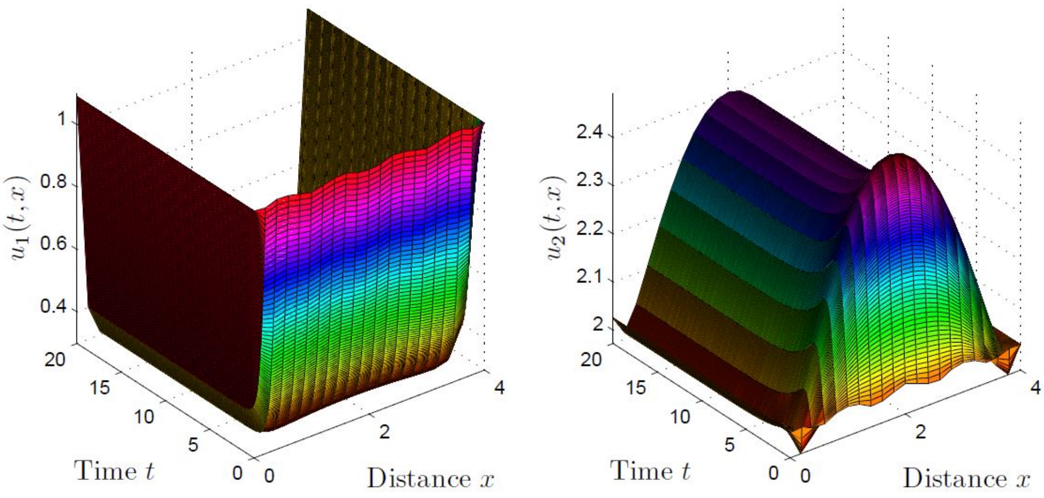

Figure 5: Approximate solution of (5)-(8), for $\alpha(t,x) = 1.35$, where $u_1 = u$ and $u_2 = v$.

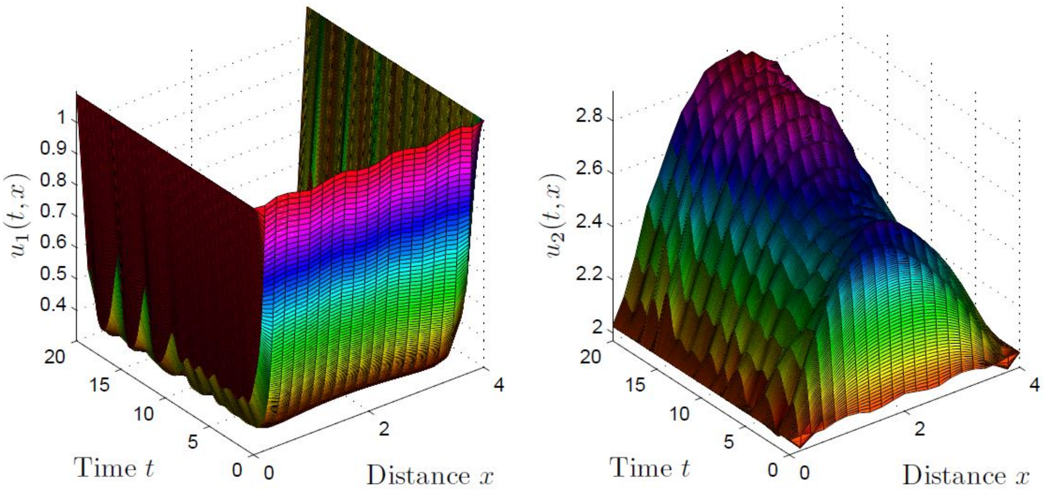

Figure 6: Approximate solution of (5)-(8), for $\alpha(t,x) = 1.5 + 0.4\cos(tx)\sin(2t)$, where $u_1 = u$ and $u_2 = v$.

7. Conclusions

In this work, we have got interesting behavior of solutions for activator-inhibitor models with variable superdiffusion by replacing the classical second derivative in space by the variable order Riesz fractional derivative of order $1 < \alpha(t,x) \leqslant 2$, it seems that our numerical results will open horizons for analytical studies about such types of models and guide them by guessing.

References

[1] S. B. Yuste, K. Lindenberg, Subdiffusion–limited reactions, Chemical physics 284 (2002) 169–180. doi:10.1016/S0301-0104(02)00546-3.

[2] D. A. Benson, S. W. Wheatcraft, M. M. Meerschaert, Application of a fractional advection–dispersion equation, Water resources research 36 (2000) 1403–1412. doi:10.1029/2000WR900031.

[3] S. B. Yuste, K. Lindenberg, Reaction front in an a+ b→ c reaction–subdiffusion process, Physical Review E 69 (2004) 036126. doi:10.1103/PhysRevE.69.036126.

[4] M. Raberto, E. Scalas, F. Mainardi, Waiting-times and returns in high-frequency financial data: an empirical study, Physica A: Statistical Mechanics and its Applications 314 (2002) 749–755. doi:10.1016/S0378-4371(02)01048-8.

[5] R. Metzler, J. Klafter, The random walk's guide to anomalous diffusion: a fractional dynamics approach, Physics reports 339 (2000) 1–77. doi:10.1016/S0370-1573(00)00070-3.

[6] Z. Hammouch, T. Mekkaoui, F. Belgacem, Numerical simulations for a variable order fractional schnakenberg model, in: AIP Conference Proceedings, American Institute of Physics, 2014, pp. 1450–1455. doi:10.1063/1.4907312.

[7] Z. Prytula, Mathematical modelling of nonlinear dynamics in activator–inhibitor systems with superdiffusion, Bulletin of the National University of Lviv Polytechnic. Computer science and information technology 826 (2015) 230–237.

[8] S. G. Samko, B. Ross, Integration and differentiation to a variable fractional order, Integral transforms and special functions 1 (1993) 277–300. doi:10.1080/10652469308819027.

[9] S. G. Samko, Fractional integration and differentiation of variable order, Analysis Mathematica 21 (1995) 213–236. doi:10.1007/bf01911126.

[10] P. Zhuang, F. Liu, V. Anh, , I. Turner, Numerical methods for the variable-order fractional advection–diffusion equation with a nonlinear source term, SIAM Journal on Numerical Analysis 47 (2009) 1760–1781. doi:10.1137/080730597.