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Numerical solution for the chemotaxis model by finite difference method

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Abstract. The finite difference method for discretization space fractional chemotaxis model is introduced in this study. The space fractional chemotaxis system is obtained from the classical advection-diffusion equations of the chemotaxis system by replacing the spatial derivative with a generalized derivative of fractional order. We compare the numerical solution of finite difference method and exact solution for a test example. The results reveal that the finite difference method is very simple and efficient for solving space fractional chemotaxis system.

1. Introduction

Chemotaxis is an important resource for cellular communication which impacts the chemical substances in the environment on the movement of mobile species. This can lead strictly oriented movement to partially oriented and partially tumbling movement. The movement towards a higher concentration of the chemical substance is called positive chemotaxis, whereas the movement towards a lower concentration is called negative chemotaxis.

The standard chemotaxis model system were described by Paltak [1], E. Keller and L. Segel [2] respectively in 1953 and 1970. It is represented by the set of partial differential equations

$$\begin{aligned} u_t - \nabla(m\nabla u) + \nabla(\xi u \nabla v) &= 0, & (x, t) \in \mathbb{R}^d \times \mathbb{R}^+, \\ \delta v_t - \Delta v + \tau v + \rho u &= 0, & (x, t) \in \mathbb{R}^d \times \mathbb{R}^+, \end{aligned} \quad (1)$$

where $u(x, t)$ denotes the density of bacteria in the position $x \in \mathbb{R}^d$ at time t , v is the concentration of chemical signal substance, $\delta \geq 0$ represents the relaxation time, the parameter ξ is the sensitivity of cells to the chemoattractant and m , τ and ρ are given smooth functions. The proposed model has been extensively studied in the last few years (see [3, 4, 5, 6, 7] for a recent survey articles).

In [8], inconsistent transport model based on space fractional differential equations is solved finite volume method. To know details about fractional Laplacian and its application, we refer



the readers to [9, 10, 11, 12, 13, 14] Recently, the fractional chemotaxis model is solved by many researchers using numerical methods [15, 16, 17].

In this paper, we considered the following space fractional chemotaxis system (SFCS):

$$u_t - D^\alpha u + \frac{\partial}{\partial x} \left(u \frac{\partial v}{\partial x} \right) = f(x, t, \alpha), \quad (x, t) \in]a, b[\times (0, T], \quad (2)$$

$$-\frac{\partial^2 v}{\partial x^2} + \tau v = 0, \quad x \in]a, b[, \quad (3)$$

with initial and boundary conditions

$$u(a, t) = u(b, t) = 0, \quad \text{for all } t \in [0, T], \quad (4)$$

$$v(a) = \gamma, \quad v(b) = \beta, \quad (5)$$

$$u(x, 0) = u_0(x), \quad \text{for all } x \in [a, b], \quad (6)$$

where $u(x, t)$ is the cell density in the position $x \in [a, b]$ at time t , v the chemical density, the function f regulates the cell death which controls the gross cell number and the positive constant τ the rate of attractant depletion, the positives constants γ and β are given and u_0 is a smooth given function. The equation (2) include the diffusion of the cells and chemotactic drift and the equation (3) expresses the production of attractant [18]. The symbol $D^\alpha u$ stands for left Riemann-Liouville fractional derivative.

Definition 1.1 (Riemann-Liouville fractional derivative on $[a, b]$ [19])

The α ($n - 1 < \alpha < n$) order left Riemann-Liouville derivative of the function on $[a, b]$ is defined as

$$D^\alpha u(x, t) = \frac{1}{\Gamma(n - \alpha)} \frac{\partial^n}{\partial x^n} \int_a^x \frac{u(\xi, t)}{(x - \xi)^{\alpha - n + 1}} d\xi = \frac{\partial^n}{\partial x^n} (I^{n - \alpha}) u(x, t), \quad (7)$$

where the function $\Gamma(\cdot)$ is the well known Gamma function and $I^\alpha(\cdot)$ is called the Riemann-Liouville integral.

If $\alpha = n$, then $D^\alpha u(x, t) = \frac{d^n u}{dx^n}$.

The numerical solution of the fractional differential equation was considered by several authors using different methods [20, 21].

In this paper, we introduce the finite difference method for solving the (SFCS) (2-6).

2. Solution methods

In this section, we only discretize the equation (2) because the equation (3) with the boundary conditions $v(a) = \gamma$ and $v(b) = \beta$ is easy to solve in the one-dimensional case and its solution is given by the following equation:

$$v(x) = A e^{\sqrt{\tau}x} + B e^{-\sqrt{\tau}x} \in C^\infty([a, b]), \quad (8)$$

where

$$A = \frac{\gamma e^{-\sqrt{\tau}b} - \beta e^{-\sqrt{\tau}a}}{e^{\sqrt{\tau}(a-b)} - e^{-\sqrt{\tau}(a-b)}}, \quad (9)$$

$$B = \frac{\beta e^{\sqrt{\tau}a} - \gamma e^{\sqrt{\tau}b}}{e^{\sqrt{\tau}(a-b)} - e^{-\sqrt{\tau}(a-b)}}. \quad (10)$$

2.1. Finite difference method

We consider a domain $[a, b]$ that is discretized with $N + 1$ uniformly spaced nodes $x_i = a + ih$ for $i = 0, \dots, N$, with the spatial step $h = (b - a)/N$. In order to numerically solve the equation (2) of the (SFCS) using the finite difference method of Meerschaert and Tadjeran [22], we first expand the advective term in (2) using the product rule.

$$\frac{\partial}{\partial x} \left[u(x, t) \frac{\partial v(x)}{\partial x} \right] = \frac{\partial u(x, t)}{\partial x} \frac{\partial v(x)}{\partial x} + \tau u(x, t) v(x). \quad (11)$$

Next, the derivative $\partial u/\partial x$ in (11) can be approximated using the central difference. This implies that a suitably one mesh is used to ensure monotonicity [23]. Now, we recall the fractional derivative Laplacian as follows:

$$D^\alpha u(x, t) = \frac{1}{\Gamma(1 - \alpha)} \frac{\partial}{\partial x} \int_a^x \frac{u(\xi, t)}{(x - \xi)^\alpha} d\xi \quad \text{for } \alpha \in]0, 1[, \quad (12)$$

$$D^\alpha u(x, t) = \frac{du(x, t)}{dx} \quad \text{for } \alpha = 1, \quad (13)$$

and

$$D^\alpha u(x, t) = \frac{1}{\Gamma(2 - \alpha)} \frac{\partial^2}{\partial x^2} \int_a^x \frac{u(\xi, t)}{(x - \xi)^{-(1+\alpha)}} \quad \text{for } \alpha \in]1, 2[. \quad (14)$$

Before discretizing the fractional Laplacian derivative, we need the following definition

Definition 2.1 (Shifted Grünwald formula on $[a, b]$ [23, 8])

$$\frac{1}{\Gamma(n - \alpha)} \frac{\partial^n}{\partial x^n} \int_a^x \frac{u(\xi, t)}{(x - \xi)^{\alpha-n+1}} d\xi \approx \frac{1}{h^\alpha} \sum_{j=0}^{[(x-a)/h+p]} w_j^\alpha u(x - (j - p)h, t), \quad (15)$$

where p is the shift value, n is the smallest integer greater than or equal to α and w_j^α are weight functions such that

$$w_0^\alpha = 1 \text{ and } w_j^\alpha = (-1)^j \frac{\alpha(\alpha - 1) \cdots (\alpha - j + 1)}{j!} \text{ for } j = 1, 2, \dots. \quad (16)$$

For $p = 0$ the equation (15) is called the standard Grünwald formula. In order to approximate the Liouville fractional derivative, we use the standard Grünwald formula for $\alpha \in]0, 1[$. However, for $\alpha \in]1, 2[$ the shift Grünwald formula for the shift $p = 1$ is required to obtain numerically stable results [22].

$$D^\alpha u(x_i, t) \approx \frac{1}{h^\alpha} \sum_{j=0}^i w_j^\alpha u(x_{i-j}, t) \quad \text{for } \alpha \in]0, 1[, \quad (17)$$

and

$$D^\alpha u(x_i, t) \approx \frac{1}{h^\alpha} \sum_{j=0}^{i+1} w_j^\alpha u(x_{i-j+1}, t) \quad \text{for } \alpha \in]1, 2[. \quad (18)$$

For the advective term, using second order central differences we can approximate the derivative of u .

$$\begin{aligned} \frac{\partial}{\partial x} u(x_i, t) \frac{\partial}{\partial x} v(x_i) + \tau u(x_i, t) v(x_i) &= \left(\frac{u(x_{i+1}, t) - u(x_{i-1}, t)}{2h} \right) \frac{\partial v(x_i)}{\partial x} \\ &+ \tau u(x_i, t) v(x_i). \end{aligned} \quad (19)$$

We now define a temporal partition $t_n = nk$ for $n = 0, 1, \dots$, where k is the time step, and approximate the temporal derivative in (19) by the standard first order backward difference. Defining $u_i^n \approx u(x_i, t_n)$ as the numerical solution, $f_i^n = f(x_i, t_n, \alpha)$ and $v_i = v(x_i)$. Then for all $\alpha \in]0, 2[$, we obtain the fully implicit scheme for the equation (19):

$$\begin{aligned} \frac{u_i^{n+1} - u_i^n}{k} &= -\frac{v'_i}{2h} (u_{i+1}^{n+1} - u_{i-1}^{n+1}) - \tau v_i u_i^{n+1} + \frac{1}{h^\alpha} \sum_{j=0}^i w_j^\alpha u_{i-j}^{n+1} + f_i^{n+1} \\ &= \sum_{j=0}^N g_{ij} u_j^{n+1} + f_j^{n+1} \quad \text{for } \alpha \in]0, 1[, \end{aligned} \quad (20)$$

$$\begin{aligned} \frac{u_i^{n+1} - u_i^n}{k} &= \frac{1 - v'_i}{2h} (u_{i+1}^{n+1} - u_{i-1}^{n+1}) - \tau v_i u_i^{n+1} + f_i^{n+1} \\ &= \sum_{j=0}^N g_{ij} u_j^{n+1} + f_j^{n+1} \quad \text{for } \alpha = 1, \end{aligned} \quad (21)$$

$$\begin{aligned} \frac{u_i^{n+1} - u_i^n}{k} &= -\frac{v'_i}{2h} (u_{i+1}^{n+1} - u_{i-1}^{n+1}) - \tau v_i u_i^{n+1} + \frac{1}{h^\alpha} \sum_{j=0}^{i+1} w_j^\alpha u_{i-j+1}^{n+1} + f_i^{n+1} \\ &= \sum_{j=0}^N g_{ij} u_j^{n+1} + f_j^{n+1} \quad \text{for } \alpha \in]1, 2[, \end{aligned} \quad (22)$$

where v'_i denotes the derivative of v at the node x_i for $i = 1, \dots, N-1$ and for $\alpha \in]0, 1[$,

$$g_{ij} = \begin{cases} h^{-\alpha} w_{i-j}^\alpha & j < i-1 \\ \frac{v'_i}{2h} + h^{-\alpha} w_1^\alpha & j = i-1 \\ -\tau v_i + h^{-\alpha} w_0^\alpha & j = i \\ -\frac{v'_i}{2h} & j = i+1 \\ 0 & j > i+1, \end{cases} \quad (23)$$

for $\alpha = 1$,

$$g_{ij} = \begin{cases} \frac{v'_{i-1}}{2h} & j = i-1 \\ -\tau v_i & j = i \\ \frac{1-v'_i}{2h} & j = i+1 \\ 0 & j > i+1 \text{ or } j < i-1, \end{cases} \quad (24)$$

for $\alpha \in]1, 2[$

$$g_{ij} = \begin{cases} w_{i-j+1}^\alpha h^{-\alpha} & j < i-1 \\ \frac{v'_i}{2h} + h^{-\alpha} w_2^\alpha & j = i-1 \\ -\tau v_i + h^{-\alpha} w_1^\alpha & j = i \\ -\frac{v'_i}{2h} + h^{-\alpha} w_0^\alpha & j = i+1 \\ 0 & j > i+1. \end{cases} \quad (25)$$

Denoting the numerical solution vector $U^n = (u_1^n, u_2^n, \dots, u_{N-1}^n)$ therefore the scheme of equation (2) was written in the matrix form as follows:

$$(I + kA) U^{n+1} = U^n + kF^{n+1}. \quad (26)$$

Remark 2.1 *As the Shifted Grünwald formula on $[a, b]$ is convergent of order 2 in space (see [23]), it is well known that the spatial derivative approximation of the function by second order central differences is again order 2 in space and the temporal derivation approximation of the function by the standard first order backward difference is order 1 in time. Then it is easy to conclude that the numerical scheme (26) is convergent of order 2 in space and order 1 in time.*

3. Results and discussions

In this section, we study the (SFCS) (2-6) for the different fractional order value $\alpha = 0.5, 1, 1.5$ and at time $T = 1$ using the finite difference method. We also compare our results with the exact solution.

Let us use the domain $[0, 50]$, the spatial step $h = 0.25$, temporal step $k = 0.005$ and $\tau = 0.01$. For this, we consider the following example:

Example:

$$u_t - D^\alpha u + \frac{\partial}{\partial x} \left(u \frac{\partial v}{\partial x} \right) = f(x, t, \alpha), \quad (x, t) \in]0, 50[\times]0, 1[, \quad (27)$$

$$-\frac{\partial^2 v}{\partial x^2} + \tau v = 0, \quad x \in]0, 50[, \quad (28)$$

with initial and boundary conditions

$$u(a, t) = u(b, t) = 0, \quad \text{for all } t \in [0, 1], \quad (29)$$

$$v(a) = 0.3, \quad v(b) = 0.2, \quad (30)$$

$$u(x, 0) = x(50 - x), \quad \text{for all } x \in [0, 50], \quad (31)$$

Here $f(t, x, \alpha) = e^{-t} [f_1(x, \alpha) - f_2(x, \alpha)]$, such that

$$\begin{aligned} f_1(x, \alpha) &= \sqrt{\tau}(50 - 2x) \left(A e^{\sqrt{\tau}x} - B e^{-\sqrt{\tau}x} \right) \\ &\quad + \tau x(50 - x) \left(A e^{\sqrt{\tau}x} + B e^{-\sqrt{\tau}x} \right) \end{aligned} \quad (32)$$

and

$$f_2(x, \alpha) = x(50 - x) + \frac{50x^{1-\alpha}}{\Gamma(2-\alpha)} - 2 \frac{x^{2-\alpha}}{\Gamma(3-\alpha)}, \quad (33)$$

where the constants A and B are defined in (9-10).

In this case, the exact solution (u, v) of the problem (41-45) is given by

$$\begin{cases} u(t, x) = x(50 - x) e^{-t} \\ v = A e^{\tau x} + B e^{-\tau x}. \end{cases} \quad (34)$$

4. Concluding remarks

In this work, the finite difference is applied for solving the space fractional chemotaxis system (SFCS) numerically. The Grünwald approach plays a key role for discretize the term of fractional derivative of the problem. This method has been examined and compared with analytic solution of the space fractional chemotaxis system. Good agreement is observed between the numerical solution obtained by the finite difference method and the analytical solution. In Biological Sciences the importance of the SFCS problem and its numerous applications, we expect to develop these results in high dimension (\mathbb{R}^2 and \mathbb{R}^3) with the temporal and spatial fractional derivative.

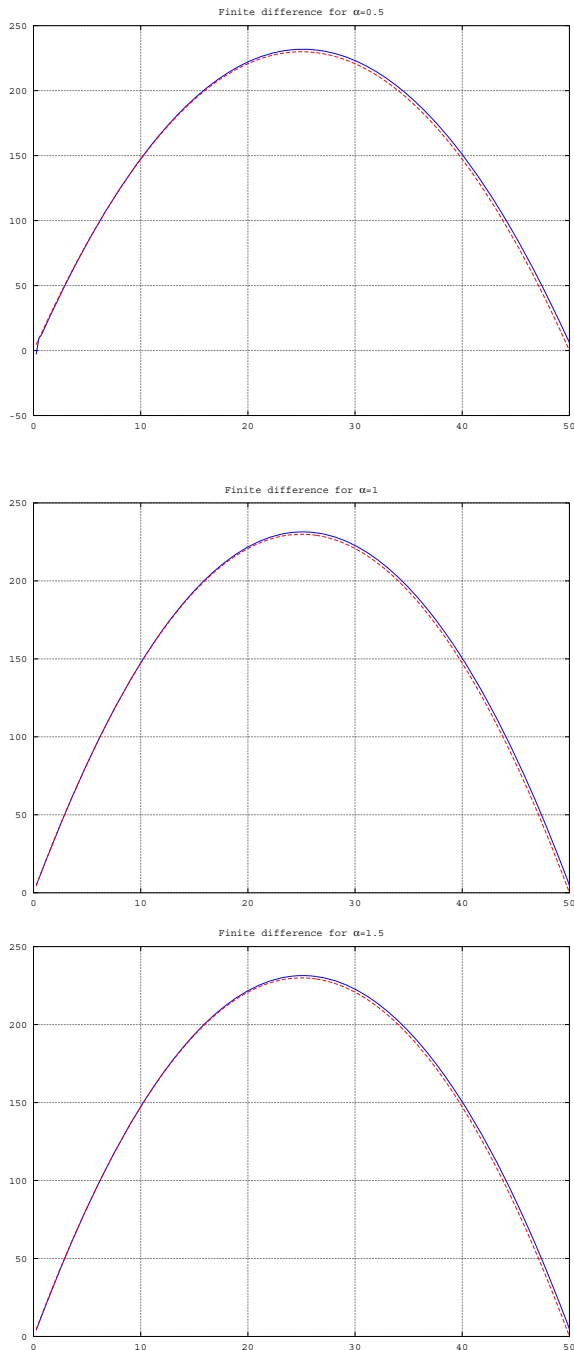


Figure 1. The finite difference method and the exact solution for different values of α . The dashed line is for the exact solution. The parameters are: $\tau = 0.01$, the time step size is 0.005, and the number of partitions of x -axis is 200.

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