Error analysis of an explicit finite difference approximation for the space fractional diffusion equation with insulated ends

S. Shen* F. Liu*†

August 25, 2004

Abstract

The space fractional diffusion equation (SFDE) is obtained from the classical diffusion equation by replacing the second space derivative by a fractional derivative of order α $(1 < \alpha \leq 2)$. Numerical methods associated with integer-order differential equations have been treated extensively in the literature. On other hand, studies of the numerical methods and error estimates of fractional order differential equations are quite limited to date. In this paper, an explicit finite difference approximation (EFDA) for SFDE is proposed. An error analysis of the explicit numerical method for SFDE with insulated ends is discussed. We derive the scaling restriction of the stability and convergence of the explicit numerical method. Finally, some numerical results are presented to show the diffusive behaviour according to the order of the space-fractional derivative and we demonstrate that our EFDA is a computationally efficient method for SFDE.

Contents

---

*School of Mathematical Sciences, Xiamen University, Xiamen 361005, China. `mailto:fwliu@xmu.edu.cn/f.liu@qut.edu.au.`

†School of Mathematical Sciences, Queensland University of Technology, QlD. 4001, Australia.

1 Introduction

Recently, fractional derivatives have found new applications in engineering, physics, finance, and hydrology [12]. The theory of fractional calculus is a useful mathematical tool for applied sciences, for example, polymer physics, biophysics and thermodynamics [4]. Nevertheless, it is somehow difficult to approximate numerically and only in the last decades researchers were motivated for the application of the associated concepts. Podlubny [13] introduced a simple, geometric interpretation of different types of fractional-order integration and proposed a physical interpretation of fractional integration in terms of an inhomogeneous and changing (non-static, dynamic) time scale. Machado [5] presented a probabilistic interpretation of the fractional-order derivative.

Space fractional diffusion equations have been investigated by West and Seshadri [14] and more recently by Gorenflo and Mainardi [2, 3]. However, numerical methods and theoretical analyses of these fractional equations are very difficult tasks. Some different numerical methods for solving fractional partial differential equation have been proposed in the literature. Liu et al. [6, 7, 8] transformed the partial differential equation into a system of ordinary differential equations (Method of Lines), which was then solved using backward differentiation formulas. Fix and Roop [1] developed a least squares finite element solution of a fractional order two-point boundary value problem. Meerschaert et al. [10] proposed finite difference approximations for fractional advection-dispersion flow equations. Lu and Liu [9] also presented explicit and implicit finite difference approximations for a space fractional advection diffusion equation and its discretization error was estimated.

In this work, we consider the space fractional diffusion equation(SFDE) with insulated ends:

$$\begin{aligned}\frac{\partial u(x,t)}{\partial t} &= d(x)\frac{\partial^\alpha u(x,t)}{\partial x^\alpha}, 0<x<L, \quad t\geq 0, \quad 1<\alpha\leq 2, & (1)\\ u(x,0) &= \psi(x), \quad 0\leq x\leq L, & (2)\\ \frac{\partial u(0,t)}{\partial x} &= 0, \quad \frac{\partial u(L,t)}{\partial x}=0, \quad t\geq 0. & (3)\end{aligned}$$

where the variable coefficient $d(x)>0$, $\frac{\partial^\alpha u(x,t)}{\partial x^\alpha}$ is the Caputo's fractional derivative ${}_0D_x^\alpha u(x)$, which is defined in [12] as

$$\frac{\partial^\alpha u}{\partial x^\alpha} = {}_a D_x^\alpha u(x) = \begin{cases} \frac{d^m u(x)}{dx^m}, & \alpha = m\in N \\ \frac{1}{\Gamma(m-\alpha)}\int_a^x (x-\xi)^{m-\alpha-1}\frac{d^m u(\xi)}{d\xi^m}d\xi, & m-1<\alpha<m \end{cases} \tag{4}$$

where $\Gamma(\cdot)$ is the Gamma function.

In this paper, an explicit finite difference approximation for the SFDE is presented. The stability and convergence of the explicit finite difference approximation are analyzed and finally, we will present some examples to show the efficiency of our numerical method.

2 An explicit finite difference approximation for SFDE

Let us suppose $h=x/k$, k is a positive integer. Using a second order difference approximation, we obtain

$$\begin{aligned} & {}_0D_x^\alpha u(x,t) \\ =\ & \frac{1}{\Gamma(2-\alpha)}\int_0^x \frac{1}{(x-\xi)^{\alpha-1}}\frac{\partial^2 u(\xi,t)}{\partial \xi^2}d\xi \\ =\ & \frac{1}{\Gamma(2-\alpha)}\sum_{j=0}^{k-1}\int_{jh}^{(j+1)h} z^{1-\alpha}\frac{\partial^2 u(x-z,t)}{\partial z^2}dz \\ \approx\ & \frac{1}{\Gamma(2-\alpha)}\sum_{j=0}^{k-1}\frac{u(x-(j-1)h,t)-2u(x-jh,t)+u(x-(j+1)h,t)}{h^2}\int_{jh}^{(j+1)h} z^{1-\alpha}dz \\ =\ & \frac{h^{-\alpha}}{\Gamma(3-\alpha)}\sum_{j=0}^{k-1}[u(x-(j-1)h,t)-2u(x-jh,t)+u(x-(j+1)h,t)] \\ & \times[(j+1)^{2-\alpha}-j^{2-\alpha}] \end{aligned} \tag{5}$$

Let $\triangle t=\tau$ be the grid step in time, $t_n=n\tau$, $0\leq t_n\leq T$, $\triangle x = h>0$ be the grid step in space, $x_j=jh$, $0\leq x_j\leq L$ for $j=0,1,\dots,K$,

$K = L/h$. Let $u_0^n = u(0, n\tau)$, $u_1^n = u(h, n\tau)$, $\cdots$, $u_{k-j}^n = u(x - jh, n\tau)$,$\cdots$,$u_j^n = u(jh, n\tau)$; $d_j = d(x_j)$; $\psi_j = \psi(x_j)$.

Now we approximate SFDE (1) using an explicit finite-difference approximation (EFDA):

$$\frac{u_k^{n+1}-u_k^n}{\tau} = d_k \frac{h^{-\alpha}}{\Gamma(3-\alpha)} \sum_{j=0}^{k-1} [u_{k-j+1}^n - 2u_{k-j}^n + u_{k-j-1}^n][(j+1)^{2-\alpha} - j^{2-\alpha}] \quad (6)$$

Eq. (6) can be rewritten in the following form:

$$u_k^{n+1} = b_k u_{k+1}^n + (1-2b_k)u_k^n + b_k u_{k-1}^n + b_k \sum_{j=1}^{k-1} g_j [u_{k-j+1}^n - 2u_{k-j}^n + u_{k-j-1}^n] \quad (7)$$

where $b_k = \frac{\tau d_k}{h^\alpha \Gamma(3-\alpha)}$, $g_k = (k+1)^{2-\alpha} - k^{2-\alpha}$.

The equations (7), together with the boundary conditions ($u_0^n = u_1^n$,$u_{K-1}^n = u_K^n$), result in the following linear system of equations:

$$U^{n+1} = AU^n \quad (8)$$

where $U^n = (u_1^n, u_2^n, \cdots, u_{K-1}^n)^T$, and $A = (a_{ij}) \in \Re^{K-1,K-1}$ is a matrix of coefficients. These coefficients, for $i = 1, 2, \cdots, K-1$ and $j = 2, 3, \cdots, K-1$ are defined as follows:

$$a_{ij} = \begin{cases} 0, & when \quad j \geq i+2, \\ b_i, & when \quad j = i+1, \\ 1 - b_i(2 - g_1), & when \quad j = i = 2, 3, \ldots, K-2, \\ b_i(1 - 2g_1 + g_2), & when \quad j = i-1, \\ b_i(g_{i-j-1} - 2g_{i-j} + g_{i-j+1}), & when \quad j \leq i-2. \end{cases} \quad (9)$$

while $a_{11} = 1 - b_1$, $a_{21} = b_2(1 - g_1)$, $a_{i1} = b_i(g_{i-2} - g_{i-1})$ for $3 \geq i \leq K-1$, $a_{K-1,K-1} = 1 - b_{K-1}(1 - g_1)$.

3 Method of Lines for SFDE

In order to demonstrate the the efficiency of the EFDA, the method of lines for SFDE also is presented. This method of lines (MoL) was firstly introduced by Liu et al. [6, 7, 8] to solve fractional partial differential equations successfully. The method of lines for SFDE can be written in the following form: for $1 < \alpha < 2$, $(k = 1, \cdots, K-1)$,

$$\frac{du_k}{dt} = b_k \sum_{j=0}^{k-1} g_j [u_{k-j+1} - 2u_{k-j} + u_{k-j-1}] \quad (10)$$

with $u_0 = u_1$, $u_K = u_{K-1}$ and $u_j = u(x_j, t)$.

4 Stability analysis of EFDA

Lemma 1: Let $A \in C^{n\times n}$ and $\rho(A)$ the spectral radius of the matrix A , then for any given positive number ε , there exists an norm $\|\cdot\|_m$ of the matrix A, such that $\|A\|_m \leq \rho(A)+\varepsilon$.

Proof. (See [9, 15]).

Theorem 1: The explicit finite-difference scheme (6) for SFDE (1)-(3) is conditionally stable.

Proof. Let λ be an eigenvalue of the matrix A in the linear system of equations (8), so that $Ax=\lambda x$ for some nonzero vector x. Choose i so that $|x_i| = max\{|x_j| : j = 1,2,\ldots,K-1\}$, then $\sum\limits_{j=1}^{K-1} a_{ij}x_j = \lambda x_i$, and therefore

$$\lambda = a_{ii} + \sum_{j=1,j\neq i}^{K-1} a_{ij}\frac{x_j}{x_i}. \tag{11}$$

Substituting the values of a_{ij} into (11) we obtain

(a) when $i=1$:

$$\lambda = 1 - b_1 + b_1\frac{x_2}{x_1} \leq 1$$

and

$$\lambda = 1 - b_1 + b_1\frac{x_2}{x_1} \geq 1 - 2b_1.$$

If $b_1 \leq 1$, we have $|\lambda| \leq 1$.

(b) when $2 \leq i \leq K-2$:

$$\begin{aligned} \lambda \;&=\; 1 - b_i(2-g_1) + b_i\tfrac{x_{i+1}}{x_i} + b_i\sum_{j=2}^{i-1}(g_{i-j-1} - 2g_{i-j} + g_{i-j+1})\tfrac{x_j}{x_i} \\ &\quad + b_i(g_{i-2} - g_{i-1})\tfrac{x_1}{x_i}. \end{aligned} \tag{12}$$

We note that $g_i > g_{i+1} > 0,\ g_{i-j-1} - 2g_{i-j} + g_{i-j+1} > 0$, for $j = 1,2,\ldots,i-1;\ i = 0,1,\ldots,K-1$, we have

$$\sum_{j=2}^{i-1}(g_{i-j-1} - 2g_{i-j} + g_{i-j+1})\frac{x_j}{x_i} \leq= g_{i-1} - g_{i-2} + g_0 - g_1$$

Since b_i are non-negative real numbers, from Eq. (12), we can get

$$\lambda \leq 1 - b_i(2-g_1) + b_i + b_i(g_{i-1} - g_{i-2} + g_0 - g_1) + b_i(g_{i-2} - g_{i-1}) = 1$$

and

$$\begin{aligned} \lambda \;&\geq\; 1 - b_i(2-g_1) - b_i - b_i(g_{i-1} - g_{i-2} + g_0 - g_1) - b_i(g_{i-2} - g_{i-1}) \\ &=\; 1 - 2b_i(2-g_1). \end{aligned}$$

If $b_i(2-g_1) \leq 1$, then $\lambda \geq -1$. Hence $|\lambda| \leq 1$.

(c) when $i = K-1$:

$$\begin{aligned} \lambda &= 1 - b_{K-1}(1-g_1) + b_{K-1}\sum_{j=2}^{K-2}(g_{K-j-2} - 2g_{K-j-1} + g_{K-j})\frac{x_j}{x_{K-1}} \\ &\quad + b_{K-1}(g_{K-3} - g_{K-2})\frac{x_1}{x_{K-1}} \end{aligned} \tag{13}$$

Thus

$$\lambda \leq 1 - b_{K-1}(1-g_1) + b_{K-1}(g_{i-1} - g_{i-2} + g_0 - g_1) + b_{K-1}(g_{i-2} - g_{i-1}) = 1$$

and

$$\begin{aligned} \lambda &\geq 1 - b_{K-1}(1-g_1) - b_{K-1}(g_{K-2} - g_{K-3} + g_0 - g_1) - b_{K-1}(g_{K-3} - g_{K-2}) \\ &= 1 - 2b_{K-1}(1-g_1). \end{aligned}$$

If $b_{K-1}(1-g_1) \leq 1$, then $\lambda \geq -1$. Hence $|\lambda| \leq 1$.

Combining (a), (b) and (c), we have that if $\max\limits_{2\leq i\leq K-2}\{b_1, b_i(2-g_1), b_{K-1}(1-g_1)\} \leq 1$, the spectral radius $\rho(A)$ of the matrix satisfies $\rho(A) \leq 1$. From Lemma 1, we get that if $\max\limits_{2\leq i\leq K-2}\{b_1, b_i(2-g_1), b_{K-1}(1-g_1)\} \leq 1$, there exists a positive number $\varepsilon \leq C\tau$, such that $\|A\|_m \leq \rho(A) + C\tau \leq 1 + O(\tau)$. Therefore, EFDA (6) is conditionally stable.

5 Convergence analysis of EFDA

Lemma 2: Let $\overline{{}_0D_x^\alpha u(x,t)} = \frac{h^{-\alpha}}{\Gamma(3-\alpha)}\sum\limits_{j=0}^{k-1} g_j[u_{k-j+1}^n - 2u_{k-j}^n + u_{k-j-1}^n]$, and $u(x,t)$ is a smooth function, then

$${}_0D_x^\alpha u(x,t) = \overline{{}_0D_x^\alpha u(x,t)} + O(h^{3-\alpha}) \tag{14}$$

Proof. (See [9, 15]).

Remark 1: The explicit finite-difference scheme (6) has a local truncation error of $e_r = O(\tau) + O(h^{3-\alpha})$.

Theorem 2: if $\max\limits_{2\leq i\leq K-2}\{b_1, b_i(2-g_1), b_{K-1}(1-g_1)\} \leq 1$, then the explicit finite-difference scheme (6) for SFDE (1)-(3) is convergence.

Proof. At the mesh points (x_k, t_n) , $y_k^n = u_k^n - e_k^n$. Substitution into (6) leads to

$$\begin{aligned} \tfrac{(u_k^{n+1} - e_k^{n+1}) - (u_k^n - e_k^n)}{\tau} &= d_k \tfrac{h^{-\alpha}}{\Gamma(3-\alpha)}\sum_{j=0}^{k-1} g_j[(u_{k-j+1}^n - 2u_{k-j}^n + u_{k-j-1}^n) \\ &\quad -(e_{k-j+1}^n - 2e_{k-j}^n + e_{k-j+1}^n)]. \end{aligned} \tag{15}$$

Using the Taylor theorem and Lemma 2, we obtain

$$\begin{aligned}[\tfrac{\partial u}{\partial t}]_k^n + O(\tau) - \tfrac{e_k^{n+1}-e_k^n}{\tau} &= d_k[\tfrac{\partial^\alpha u}{\partial x^\alpha} + O(h^{3-\alpha})] \\ &\quad -\tfrac{d_k h^{-\alpha}}{\Gamma(3-\alpha)} \sum_{j=0}^{k-1} g_j(e_{k-j+1}^n - 2e_{k-j}^n + e_{k-j-1}^n).\end{aligned} \tag{16}$$

Thus, we have

$$\tfrac{e_k^{n+1}-e_k^n}{\tau} = \tfrac{d_k h^{-\alpha}}{\Gamma(3-\alpha)} \sum_{j=0}^{k-1} g_j(e_{k-j+1}^n - 2e_{k-j}^n + e_{k-j-1}^n) + [O(\tau) + O(h^{3-\alpha})]. \tag{17}$$

Using the initial and boundary conditions $e_k^0 = 0$, $e_0^{n+1} = e_1^{n+1}$, $e_{K-1}^{n+1} = e_K^{n+1}$, Eq. (16) can be rewritten in matrix form:

$$E_{n+1} = AE_n + M \quad , \quad E_0 = 0 \tag{18}$$

where $E_n = (e_1^n, e_2^n, \cdots, e_{K-1}^n)^T$, $M = \tau(O(\tau) + O(h^{3-\alpha}))(1, 1, \cdots, 1)^T$.

Hence, we obtain

$$E_{n+1} = (A^n + A^{n-1} + \cdots + A^2 + A + I)M \tag{19}$$

Thus

$$\|E_{n+1}\|_\infty \leq (\|A^n\|_\infty + \|A^{n-1}\|_\infty + \cdots + \|A\|_\infty + \|I\|_\infty)\|M\|_\infty. \tag{20}$$

Because

$$\begin{aligned} & \|A\|_\infty = \max_{1\leq i\leq K-1} \sum_{j=1}^{K-1} |a_{ij}| \\ = \; & \max\{|1-b_1| + b_1, \max_{2\leq i\leq K-1}[|1-b_i(2-g_1)| + b_i(2-g_1)], \\ & |1-b_{K-1}(1-g_1)| + b_{K-1}(1-g_1)\} \end{aligned}$$

If $\max\limits_{2\leq i\leq K-2}\{b_1, b_i(2-g_1), b_{K-1}(1-g_1)\} \leq 1$, then $\|A\|_\infty \leq 1$. Thus, we obtain

$\|E_{n+1}\|_\infty \leq (n+1)\tau|O(\tau) + O(h^{3-\alpha})|$.

Consequently, when $\tau \to 0$, $h \to 0$, we have $\|E_{n+1}\|_\infty \to 0$, i.e. $|e_k^{n+1}| \to 0$. This proves that y converges to u as τ and h tends to zero if $\max\limits_{2\leq i\leq K-2}\{b_1, b_i(2-g_1), b_{K-1}(1-g_1)\} \leq 1$.

6 Numerical results

In this section, the following space fractional diffusion equation(SFDE) with insulated ends is considered:

$$\frac{\partial u(x,t)}{\partial t} = d\frac{\partial^{\alpha}u(x,t)}{\partial x^{\alpha}}, 0<x<\pi, \quad t\geq 0, \quad 1<\alpha\leq 2, \tag{21}$$

$$u(x,0) = \psi(x)=x^2, \quad 0\leq x\leq \pi, \tag{22}$$

$$\frac{\partial u(0,t)}{\partial x} = 0, \quad \frac{\partial u(\pi,t)}{\partial x}=0, \quad t\geq 0. \tag{23}$$

When $\alpha=2$, d constant, the analytical solution of the heat equation with insulated ends [11] is

$$u(x,t)=\frac{1}{3}\pi^2+\sum_{n=1}^{\infty}(\frac{4(-1)^n}{n^2})\cos(nx)e^{-n^2dt}. \tag{24}$$

In Figure 1, the analytical solution, numerical solutions (MoL) and EFDA for $\alpha=2$, $d=0.4$, $t=0.3$ are shown. From Figure 1, it can be seen that both numerical solutions are in good agreement with the analytical solution.

In Figure 2, the numerical solutions using MoL and EFDA with $h=\pi/100$, $\tau=0.0001$ for $\alpha=1.7$, $d=0.4$, $t=0.3$ are shown. From Figure 2, it can be seen that EFDA is in good agreement with MoL. The EFDA is an explicit and is computationally simple. It can demonstrate that our EFDA is an computationally efficient method for SFDE.

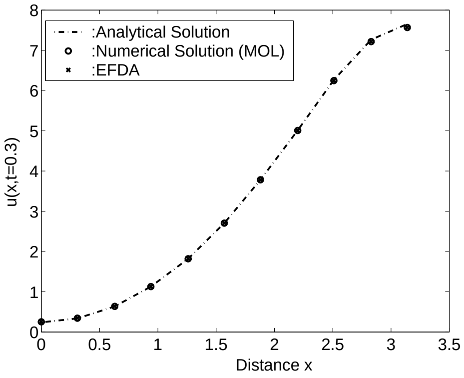

Figure 1: The analytical solution, numerical solutions (MoL) and EFDA for $\alpha=2$, $d=0.4$, $t=0.3$.

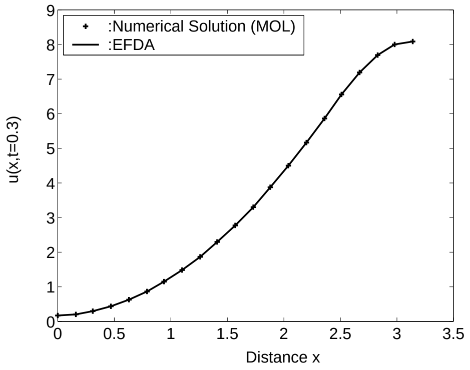

Figure 2: The numerical solutions using MoL and EFDA with $h=\pi/100$, $\tau=0.0001$ respectively for $\alpha=1.7$, $d=0.4$, $t=0.3$.

Figure 3 shows the evolution result using EFDA with $h=\pi/100$, $\tau=0.0001$, $\alpha=1.7$ ($0\leq t\leq 1$, $0\leq x\leq \pi$). It can be seen that the $\alpha=1.7$ order derivative system exhibits diffusive behaviour with different times.

Figure 4 compares the response of the diffusion system using EFDA for different real numbers $1.5 \leq \alpha \leq 2$. From Figure 4, it can be seen that the diffusive behaviour according to the order of the space-fractional derivative.

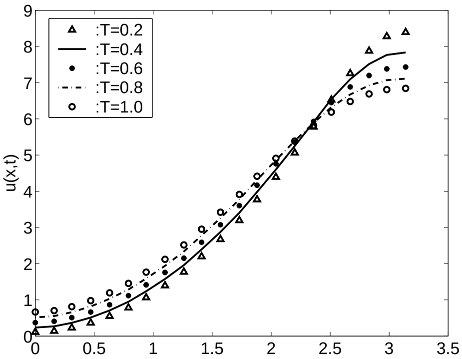

Figure 3: The evolution result using EFDA with $h = \pi/100$, $\tau = 0.0001$, $\alpha = 1.7$ $(0 \leq t \leq 1,\ 0 \leq x \leq \pi)$.

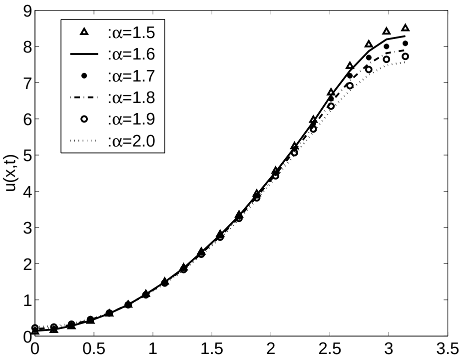

Figure 4: Compare the response of the diffusion system using EFDA for different real numbers $1.5 \leq \alpha \leq 2$.

7 Conclusion

In this paper, an explicit finite difference approximation (EFDA) for SFDE is presented. The error analysis, stability and convergence of the explicit numerical method for SFDE with insulated ends are discussed. Finally, some numerical results are presented to demonstrate that our EFDA is a computationally efficient method for SFDE. This method can be applied to solve fractional differential equations.

References

[1] G.J. Fix and J.P. Roop, Least squares finite element solution of a fractional order two-point boundary value problem, Comput. Math. Appl. 2003, to appear.

[2] R. Gorenflo and F. Mainardi, Random Walk Models for Space Fractional Diffusion Processes, Frac. Cal. Appl. Anal. 1, 1998, 167-191.

[3] R. Gorenflo and Mainardi,F., Approximation of Levy-Feller Diffusion by Random Walk, Journal for Analysis and its Applications (ZAA) 18, 1999, 231-246.

[4] R. Hilfer, Application of fractional calculus in physics, World Scientific, 2000.

[5] J.A. Tenreiro Machado, A Probabilistic Interpretation of the Fractional-Order Differentiation, Fractional Calculus & Applied Analysis, 6, No 1 (2003), 73-80.

[6] F. Liu, V. Anh and I. Turner, Numerical solution of the fractional-order Advection-Dispersion Equation, The Procceding of An International Conference on Boundary and Interior Layers -Computational and Asymptotic Methods, Perth, Australia, 159-164, 2002.

[7] F. Liu, V. Anh, I. Turner, Numerical Solution of the Space Fractional Fokker-Planck Equation, Journal of Computational and Applied Mathematics 166, 2004, 209-219.

[8] F. Liu, V. Anh, I. Turner and P. Zhuang, Numerical simulation for solute transport in fractal porous media, ANZIAM J., 45(E) 461-473, 2004.

[9] X. Lu and F. Liu, The explicit and implicit finite difference approximations for a space fractional advection diffusion equation, Computational Mechanics, WCCM VI in conjuncton with APCOM'04, 2004, to appear.

[10] M.M. Meerschaert and C. Tadjeran, Finite difference approximations for fractional advection-dispersion flow equations, Journal of Computational and Applied Mathematics, 2004, to appear.

[11] P.V. O'Neil, Advanced Engineering Mathematics, Thomson Brooks/Cole, 2003.

[12] I. Podlubny, Fractional Differential Equations, Academic, Press, New York, 1999.

[13] I. Podlubny, Geometric and Physical Interpretation of Fractional Integration and Fractional Differentiation, Fractional Calculus & Applied Analysis, 5, No 4 (2002), 367-386.

[14] B. West and V. Seshadri, Linear Systems With Levy Fluctuations, Physica A 113, 1982, 203-216.

[15] Z. Xu, K. Zhang, Q. Lu, G. Leng, Matrix Theory, Scientific publishing house, 2001.