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NUMERICAL SOLUTIONS TO BOUNDARY VALUE PROBLEM FOR ANOMALOUS DIFFUSION EQUATION WITH RIESZ-FELLER FRACTIONAL OPERATOR

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In this paper, we present a numerical solution to an ordinary differential equation of a fractional order in one-dimensional space. The solution to this equation can describe a steady state of the process of anomalous diffusion. The process arises from interactions within complex and non-homogeneous background. We present a numerical method which is based on the finite differences method. We consider a boundary value problem (Dirichlet conditions) for an equation with the Riesz-Feller fractional derivative. In the final part of this paper, some simulation results are shown. We present an example of non-linear temperature profiles in nanotubes which can be approximated by a solution to the fractional differential equation.

Key words: Riesz-Feller fractional derivative, boundary value problem, Dirichlet conditions, finite difference method

1. Introduction

Anomalous diffusion is a phenomenon strongly connected with interactions within complex and non-homogeneous background. This phenomenon is observed in transport of a fluid in porous materials, in chaotic heat baths, amorphous semiconductors, particle dynamics inside a polymer network, two-dimensional rotating flow and also in econophysics. The phenomenon of anomalous diffusion deviates from the standard diffusion behaviour. In opposite to the standard diffusion where a linear form in the mean square displacement $\langle x^2(t)\rangle \sim k_1 t$ of the diffusing particle over time occurs, the anomalous diffusion is characterized by a non-linear one $\langle x^2(t)\rangle \sim k_\gamma t^\gamma$, for $\gamma \in (0,2]$. In this phenomenon, there may exist a dependence $\langle x^2(t) \rangle \to \infty$ characterized by occurrence of rare but extremely large jumps of diffusing particles – well-known as the Levy motion or the Levy flights. An ordinary diffusion follows Gaussian statistics and Fick's second law for finding the running process at time t whereas anomalous diffusion follows non-Gaussian statistics or can be interpreted as the Levy stable densities.

Many authors proposed models which base on linear and non-linear forms of differential equations. Such models can simulate anomalous diffusion but they do not reflect its real behaviour. Several authors (Carpinteri and Mainardi, 1997; Hilfer, 2000; Gorenflo and Mainardi, 1998; Metzler and Klafter, 2000) apply fractional calculus to the modelling of this type of diffusion. This means that time and spatial derivatives in the classical diffusion equation are replaced by fractional ones. In comparison to derivatives of the integer order, which depend on the local behaviour of the function, the derivatives of the fractional order accumulate the whole history of this function.

In our previeus works (Ciesielski and Leszczynski, 2003, 2005), we presented a solution to a partial differential equation of the fractional order with the time fractional operator and the space ordinary operator, respectively. Those solutions were based on the Finite Difference Method (FDM) and are called the Fractional FDM (FFDM).

2. Mathematical background

In this paper we consider an ordinary differential equation of fractional order in the following form

$$\frac{d^\alpha}{d|x|^\alpha_\theta} T(x) = 0 \qquad x \in \mathbb{R} \tag{2.1}$$

where $T(x)$ is a field variable (i.e. field temperature), $(d^\alpha / d|x|^\alpha_\theta) T(x)$ is the Riesz-Feller fractional operator (Metzer and Klafter, 2000; Samko *et al.*, 1993), α is the real order of this operator and θ is the skewness parameter. According to (Gorenflo and Mainardi, 1998), the Riesz-Feller fractional operator is defined as

$$\frac{d^\alpha}{d|x|^\alpha_\theta} T(x) = {}_x D^\alpha_\theta T(x) = -[c_L(\alpha,\theta)\, {}_{-\infty}D^\alpha_x T(x) + c_R(\alpha,\theta)\, {}_x D^\alpha_{+\infty} T(x)] \tag{2.2}$$

for $0 < \alpha \leqslant 2,\ \alpha \neq 1$ where

$$
\begin{aligned}
{}_{-\infty}D_x^{\alpha}T(x) &= \Big(\frac{d}{dx}\Big)^m [{}_{-\infty}I_x^{m-\alpha}T(x)] \\
{}_xD_{+\infty}^{\alpha}T(x) &= (-1)^m\Big(\frac{d}{dx}\Big)^m [{}_xI_{+\infty}^{m-\alpha}T(x)]
\end{aligned}
\tag{2.3}
$$

for $m \in \mathbb{N}$, $m-1 < \alpha \leqslant m$, and the coefficients $c_L(\alpha,\theta)$, $c_R(\alpha,\theta)$ (for $0 < \alpha \leqslant 2$, $\alpha \neq 1$, $|\theta| \leqslant \min(\alpha, 2-\alpha)$) are defined as

$$
c_L(\alpha,\theta) = \frac{\sin\frac{(\alpha-\theta)\pi}{2}}{\sin(\alpha\pi)} \qquad\qquad c_R(\alpha,\theta) = \frac{\sin\frac{(\alpha+\theta)\pi}{2}}{\sin(\alpha\pi)}
\tag{2.4}
$$

The fractional integral operators of the order α: ${}_{-\infty}I_x^{\alpha}T(x)$ and ${}_xI_{\infty}^{\alpha}T(x)$ are defined as the left- and right-hand of Weyl's fractional integrals (Carpinteri and Mainardi, 1997; Oldham and Spaner, 1974; Podlubny, 1999; Samko *et al.*, 1993) whose definitions are

$$
\begin{aligned}
{}_{-\infty}I_x^{\alpha}T(x) &= \frac{1}{\Gamma(\alpha)}\int\limits_{-\infty}^{x} \frac{T(\xi)}{(x-\xi)^{1-\alpha}}\,d\xi \\
{}_xI_{\infty}^{\alpha}T(x) &= \frac{1}{\Gamma(\alpha)}\int\limits_{x}^{\infty} \frac{T(\xi)}{(\xi-x)^{1-\alpha}}\,d\xi
\end{aligned}
\tag{2.5}
$$

Considering Eq. (2.1), we obtain the steady state of the classical diffusion equation for $\alpha = 2$, i.e. the heat transfer equation. If $\alpha = 1$, and the parameter of skewness θ admits extreme values in (2.4), the steady state of a transport equation is noted. Therefore we assume variations of the parameter α within the range $0 < \alpha \leqslant 2$. Analysing behaviour of the parameter $\alpha < 2$ in Eq. (2.1), we found some combination between transport and propagation processes in steady states.

In this work, we will consider equation (2.1) in one dimensional domain $\Omega : L \leqslant x \leqslant R$ with boundary-value conditions of the first kind (Dirichlet conditions) as

$$
\begin{cases}
x = L: & T(L) = g_L \\
x = R: & T(R) = g_R
\end{cases}
\tag{2.6}
$$

3. Numerical method

According to the finite difference method (Hoffman, 1992; Majchrzak and Mochnacki, 1996), we consider a discrete from of equation (2.1) in space. The problem of solving equation (2.1) lies in a proper approximation of Riesz-Feller derivative (2.2) by a numerical scheme.

3.1. Approximation of the Riesz-Feller derivative

In order to develop a discrete form of operator (2.2), we introduce a homogenous spatial grid $-\infty < \ldots < x_{i-2} < x_{i-1} < x_i < x_{i+1} < x_{i+2} < \ldots < \infty$ with the step $h = x_k - x_{k-1}$. We denote a value of the function T in the point x_k as $T_k = T(x_k)$, for $k \in \mathbb{Z}$. For the numerical integration scheme, we assumed the trapezoidal rule and we used various weighted numerical differential schemes for the first and second derivatives, respectively. The method of determination of the discrete form of this operator was described in detail in work by Ciesielski (2005) and its final form is the following

$$
{}_{x_i}D^{\alpha}_{\theta} T_i \approx \frac{1}{h^{\alpha}} \sum_{k=\infty}^{\infty} T_{i+k} w_k^{(\alpha,\theta)} \tag{3.1}
$$

where coefficients $w_k^{(\alpha,\theta)}$, for $0 < \alpha < 1$, have the form

$$
\begin{aligned}
w_k^{(\alpha,\theta)} = {} & \frac{-1}{2\Gamma(2-\alpha)} \cdot \\
& \cdot \begin{cases}
[(|k|+2)^{1-\alpha}\lambda_1 + (|k|+1)^{1-\alpha}(2-3\lambda_1) + \\
\quad + |k|^{1-\alpha}(3\lambda_1 - 4) + (|k|-1)^{1-\alpha}(2-\lambda_1)]c_L & \text{for} \quad k \leqslant -2 \\
[3^{1-\alpha}\lambda_1 + 2^{1-\alpha}(2-3\lambda_1) + 3\lambda_1 - 4]c_L + \lambda_1 c_R & \text{for} \quad k = -1 \\
(2^{1-\alpha}\lambda_1 - 3\lambda_1 + 2)(c_L + c_R) & \text{for} \quad k = 0 \\
[3^{1-\alpha}\lambda_1 + 2^{1-\alpha}(2-3\lambda_1) + 3\lambda_1 - 4]c_R + \lambda_1 c_L & \text{for} \quad k = 1 \\
[(k+2)^{1-\alpha}\lambda_1 + (k+1)^{1-\alpha}(2-3\lambda_1) + \\
\quad + k^{1-\alpha}(3\lambda_1 - 4) + (k-1)^{1-\alpha}(2-\lambda_1)]c_R & \text{for} \quad k \geqslant 2
\end{cases}
\end{aligned} \tag{3.2}
$$

and for $1 < \alpha \leqslant 2$, we obtain

$$w_k^{(\alpha,\theta)} = \frac{-1}{2\Gamma(3-\alpha)} \cdot \begin{cases} [(|k|+2)^{2-\alpha}(2-\lambda_2) + (|k|+1)^{2-\alpha}(4\lambda_2-6)+ \\ \quad + |k|^{2-\alpha}(6-6\lambda_2) + (|k|-1)^{2-\alpha}(4\lambda_2-2)+ \\ \quad + (|k|-2)^{2-\alpha}(-\lambda_2)]c_L & \text{for} \quad k \leqslant -2 \\ [3^{2-\alpha}(2-\lambda_2) + 2^{2-\alpha}(4\lambda_2-6) - 6\lambda_2 + 6]c_L+ \\ \quad + (2-\lambda_2)c_R & \text{for} \quad k = -1 \\ [2^{2-\alpha}(2-\lambda_2) + 4\lambda_2 - 6](c_L + c_R) & \text{for} \quad k = 0 \\ [3^{2-\alpha}(2-\lambda_2) + 2^{2-\alpha}(4\lambda_2-6) - 6\lambda_2 + 6]c_R+ \\ \quad + (2-\lambda_2)c_L & \text{for} \quad k = 1 \\ [(k+2)^{2-\alpha}(2-\lambda_2) + (k+1)^{2-\alpha}(4\lambda_2-6)+ \\ \quad + k^{2-\alpha}(6-6\lambda_2) + (k-1)^{2-\alpha}(4\lambda_2-2)+ \\ \quad + (k-2)^{2-\alpha}(-\lambda_2)]c_R & \text{for} \quad k \geqslant 2 \end{cases} \tag{3.3}$$

Assuming $\alpha = 2$, $\theta = 0$ and $c_L(2,0) = c_R(2,0) = -1/2$, we obtain

$$w_k^{(2,0)} = \begin{cases} 0 & \text{for} \quad k \leqslant -2 \\ 1 & \text{for} \quad k = -1 \\ -2 & \text{for} \quad k = 0 \\ 1 & \text{for} \quad k = 1 \\ 0 & \text{for} \quad k \geqslant 2 \end{cases} \tag{3.4}$$

These coeeficients are identical as in the well known central difference scheme for the second derivative.

The authors did not find exact values of the approximating coefficients in literature. When $\alpha = 1$, the Riesz-Feller operator is singular, hence the problem occurs.

3.2. Fractional FDM

Having the discretization of the Riesz-Feller derivative in space done, in this subsection we describe the finite difference method for equation (2.1). Here we restrict the solution to one dimensional space in comparison with the standard diffusion equation where the discretization of the second derivative in space can approximate the central difference of the second order. The differences appear in the setting of boundary conditions.

In the scheme of FDM, we replaced equation (2.1) by the following formula

$$\frac{1}{h^\alpha}\sum_{k=-\infty}^{\infty} T_{i+k} w_k^{(\alpha,\theta)} = 0 \tag{3.5}$$

Here, for the unbounded domain we are obliged to solve a system of algebraic equations with an infinite dimension.

3.2.1. Boundary value problem

Present numerical scheme (3.5) with the included unbounded domain $-\infty < x < \infty$ has no practical implementations to computer simulations.

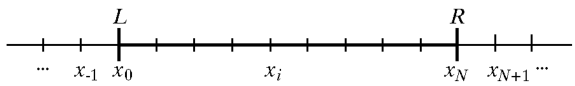

Fig. 1. Spatial distribution of grid nodes

Now we show solution to this problem on the finite domain $\Omega :\ L \leqslant x \leqslant R$ with boundary conditions (2.6). We divide domain Ω into N sub-domains with $h = (R-L)/N$. Figure 1 shows a modified spatial grid. Here we can observe additional 'virtual' points in the grid placed outside the domain Ω. In order to introduce the Dirichlet boundary conditions, we proposed a treatment which is based on the assumption that values of the function T in outside points are identical with values in the boundary nodes x_0 or x_N

$$T(x_k) = \begin{cases} T(x_0) = g_L & \text{for} \quad k < 0 \\ T(x_N) = g_R & \text{for} \quad k > N \end{cases} \tag{3.6}$$

On the basis of above considerations, we modify expression (3.1) for the discretization of the Riesz-Feller derivative. Thus we have

$${}_{x_i}D_\theta^\alpha T(x_i) \approx \frac{1}{h^\alpha}\Big(\sum_{k=-i}^{N-i} T_{i+k} w_k^{(\alpha,\theta)} + g_L s_{L_i}^{(\alpha,\theta)} + g_R s_{R_{N-i}}^{(\alpha,\theta)}\Big) \tag{3.7}$$

for $i = 1,\dots,N-1$, where

$$\begin{aligned} s_{L_j}^{(\alpha,\theta)} &= \sum_{k=-\infty}^{-j-1} w_k^{(\alpha,\theta)} = \begin{cases} c_L(\alpha,\theta)\widetilde{r}_j & \text{for} \quad 0 < \alpha < 1 \\ c_L(\alpha,\theta)\widetilde{\widetilde{r}}_j & \text{for} \quad 1 < \alpha \leqslant 2 \end{cases} \\ s_{R_j}^{(\alpha,\theta)} &= \sum_{k=j+1}^{\infty} w_k^{(\alpha,\theta)} = \begin{cases} c_R(\alpha,\theta)\widetilde{r}_j & \text{for} \quad 0 < \alpha < 1 \\ c_R(\alpha,\theta)\widetilde{\widetilde{r}}_j & \text{for} \quad 1 < \alpha \leqslant 2 \end{cases} \end{aligned} \tag{3.8}$$

and

$$\widetilde{r}_j = \frac{(j+2)^{1-\alpha}\lambda_1 + (j+1)^{1-\alpha}(2-2\lambda_1) + j^{1-\alpha}(\lambda_1 - 2)}{2\Gamma(2-\alpha)}$$

$$\widetilde{\widetilde{r}}_j = \frac{(j+2)^{2-\alpha}(2-\lambda_2) + (j+1)^{2-\alpha}(3\lambda_2 - 4) + j^{2-\alpha}(2-3\lambda_2)}{2\Gamma(3-\alpha)} + \\ + \frac{(j-1)^{2-\alpha}\lambda_2}{2\Gamma(3-\alpha)} \tag{3.9}$$

Putting expression (3.7) to equation (2.1), we obtain the following finite difference scheme

$$\sum_{k=-i}^{N-i} T_{i+k} w_k^{(\alpha,\theta)} + g_L s_{L_i}^{(\alpha,\theta)} + g_R s_{R_{N-i}}^{(\alpha,\theta)} = 0 \qquad i = 0, \dots, N \\ T_0 = g_L \qquad T_N = g_R \tag{3.10}$$

The above scheme described by expression (3.12) can be written in a matrix form as

$$\mathsf{A} \cdot \boldsymbol{T} = \boldsymbol{B} \tag{3.11}$$

where

$$\mathsf{A} = \begin{bmatrix} 1 & 0 & 0 & 0 & \dots & 0 & 0 & 0 \\ a_{-1} & a_0 & a_1 & a_2 & \dots & a_{N-3} & a_{N-2} & a_{N-1} \\ a_{-2} & a_{-1} & a_0 & a_1 & \dots & a_{N-4} & a_{N-3} & a_{N-2} \\ a_{-3} & a_{-2} & a_{-1} & a_0 & \dots & a_{N-5} & a_{N-4} & a_{N-2} \\ a_{-4} & a_{-3} & a_{-2} & a_{-1} & \dots & a_{N-6} & a_{N-3} & a_{N-4} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ a_{-N+2} & a_{-N+3} & a_{-N+4} & a_{-N+5} & \dots & a_0 & a_1 & a_2 \\ a_{-N+1} & a_{-N+2} & a_{-N+3} & a_{-N+4} & \dots & a_{-1} & a_0 & a_1 \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & 1 \end{bmatrix} \\ \boldsymbol{B} = [g_L, b_1, b_2, b_3, b_4, \dots, b_{N-2}, b_{N-1}, g_R]^\top \tag{3.12}$$

with

$$a_j = w_j^{(\alpha,\theta)} \qquad \text{for} \quad j = -N+1, \dots, N-1 \\ b_j = g_L s_{L_j}^{(\alpha,\theta)} + g_R s_{R_j}^{(\alpha,\theta)} \qquad \text{for} \quad j = 1, \dots, N-1 \tag{3.13}$$

and $\boldsymbol{T} = [T_0, T_1, T_2, \dots, T_N]^\top$ is the vector of unknown values of the function T.

We can observe that the boundary conditions influence all values of the function in every node. In opposite to the second derivative over space, which is approximated locally, the characteristic feature of the Riesz-Feller and other fractional derivatives is the dependence on values of all domain points. For $\alpha = 2$ and $\theta = 0$, our scheme is identical as with the well known and used central difference scheme in space (Hoffman, 1992; Majchrzak and Mochnacki, 1996).

The skewness parameter θ has significant influence on the solution. For $\alpha \to 1^+$ and $\theta \to \pm 1^+$ one can obtain the classical ordinary differential equation.

4. Simulation results

In this section, we present results of calculation. In all presented simulations we assumed $0 \leqslant x \leqslant 1$. Figure 2 shows temperature profiles over space with boundary conditions $g_L = 2$, $g_R = 1$ for different values $\alpha = \{0.1, 0.5.0.75, 1.01, 1.25, 1.5, 1.75, 2\}$ and $\theta = 0$. Figure 3 presents another example of the solution in which we assumed $\alpha = 1.01$ and different values of the skewness parameter $\theta = \{0, 0.1, 0.3, 0.5, 0.7, 0.9, 0.99\}$.

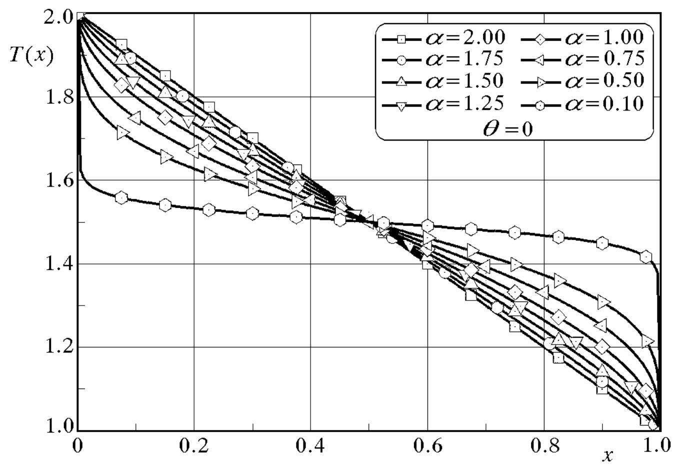

Fig. 2. Spatial solution to equation (2.1) for different values of α and $\theta = 0$

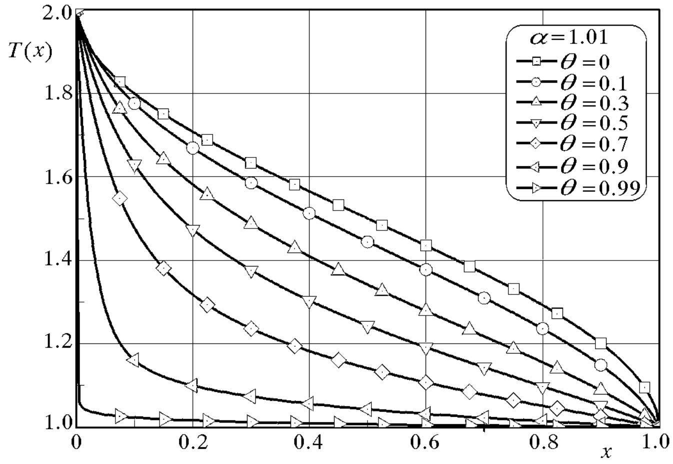

Fig. 3. Spatial solution to equation (2.1) for a steady value of the parameter $\alpha = 1.01$ and different values of $\theta = 0$

The last example illustrates the heat transport in nanotubes. Figure 4 presents experimental data prerformed by Zhang and Li (2005) and results of our numerical solution of equation (2.1). For such a comparison we assumed $\alpha = 0.35$ and $\theta = -0.055$ to best fit the experimental data. It should be noted that the temperature profile inside the nanotube deviates from the profile obtained by solving the standard heat transfer equation.

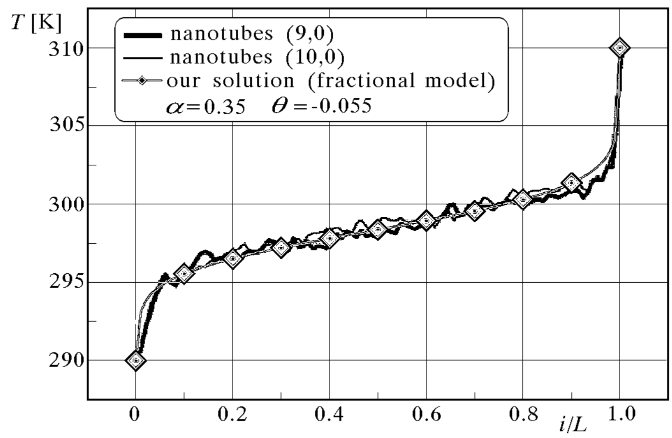

Fig. 4. Comparison of temperature profiles in nanotubes measured by Zhang and Li (2005) and obtained by numerical solution to equation (2.1)

5. Conclusions

Summing up, we proposed a fractional finite difference method for the fractional diffusion equation with the Riesz-Feller fractional derivative which is an extension of the standard diffusion. We analysed a linear case of the steady state of the anomalous diffusion equation, and in the future we will work on non-linear cases. We obtained the FDM scheme which generalises classical scheme of FDM for the diffusion equation. Moreover, for $\alpha = 2$, our solution is equivalent with that obtained by the classical finite difference method.

Analysing plots included in this work, we can see that in the case $\alpha = 2$, solution of Eq. (2.1) is a linear function. In the other cases, when $\alpha < 2$, solutions are non-linear functions. When we analyse the probability density function generated by fractional diffusion equation for $\alpha < 2$, we observe a long tail of distribution. In this way we can simulate same rare and extreme events which are characterised by arbitrary very large values of particle jumps.

Analysing the changes in the skewness parameter θ, we observed interesting behaviour in the solution. For $\alpha \to 1^+$ and for $\theta \to \pm 1^+$, we obtained the steady state of the first order wave equation. For $\theta \in (0,1)$ (with restrictions to the order α), we generated non-symmetric solutions. It should be noted that we can good approximate the temperature profile inside the nanotubes using solution of Eq. (2.1).

References

1. Carpinteri A., Mainardi F. (eds.), 1997, *Fractals and Fractional Calculus in Continuum Mechanics*, Springer Verlag, Vienna-New-York
2. Ciesielski M., 2005, *Fractional finite difference method applied for solution of anomalous diffusion equations with initial-boundary conditions*, PhD Thesis, Czestochowa, (in Polish)
3. Ciesielski M., Leszczynski J., 2003, Numerical simulations of anomalous diffusion, *Proc. 15th International Conference on Computer Methods in Mechanics CMM-2003*, 1-5 (proceeding on CD-ROM)
4. Ciesielski M., Leszczynski J., 2005, Numerical solutions of a boundary value problem for the anomalous diffusion equation with the Riesz fractional derivative, *Proc. 16th International Conference on Computer Methods in Mechanics CMM-2005*, 1-5 (proceeding on CD-ROM)

5. Gorenflo R., Mainardi F., 1998, Fractional calculus and stable probability distributions, *Archives of Mechanics*, **50**, 3, 377-388

6. Hilfer R., 2000, *Applications of Fractional Calculus in Physics*, World Scientific Publ. Co., Singapore

7. Hoffman J.D., 1992, *Numerical Methods for Engineers and Scientists*, McGraw-Hill

8. Majchrzak E., Mochnacki B., 1996, *Metody numeryczne, Podstawy teoretyczne. Aspekty praktyczne i algorytmy*, Wydawnictwo Politechniki Slaskiej (in Polish), Gliwice

9. Metzler R., Klafter J., 2000, The random walk's guide to anomalous diffusion: a fractional dynamics approach, *Phys. Rep.*, **339**, 1-70

10. Oldham K., Spanier J., 1974, *The Fractional Calculus*, Academic Press, New York and London

11. Podlubny I., 1999, *Fractional Differential Equations*, Academic Press, San Diego

12. Samko S.G., Kilbas A.A., Marichev O.I., 1993, *Integrals and Derivatives of Fractional Order and Same of their Applications*, Gordon and Breach, London

13. Zhang G., Li B., 2005, Thermal conductivity of nanotubes revisited: Effects of chirality, isotope impurity, tube length, and temperature, *J. Chem. Phys.*, **123**, 114714

Numeryczne rozwiązanie zagadnienia brzegowego równania anomalnej dyfuzji z operatorem frakcjalnym Riesza-Fellera

Streszczenie

W pracy zaprezentowano numeryczne rozwiązanie jednowymiarowego równania różniczkowego zwyczajnego niecałkowitego rzędu. Rozwiązanie tego równania może opisywać stan ustalony procesu anomalnej dyfuzji. Proces ten wynika z oddziaływań zachodzących w złożonych i niejednorodnych systemach. Zaprezentowana metoda numeryczna oparta jest na metodzie różnic skończonych. Rozważane było zagadnienie brzegowe z warunkami Dirichleta dla tego równania z pochodną frakcjalną Riesza-Fellera. W końcowej części przedstawiono wyniki symulacji. Jako przykład zaprezentowano nieliniowy profil temperatury w nanorurkach, który może być przybliżony przez rozwiązanie frakcjalnego równania różniczkowego.

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