A finite element solution for the fractional equation*

Petra Nováčková[†], Tomáš Kisela

Brno University of Technology, Brno, Czech Republic

Abstract

This contribution presents a numerical method for solving diffusion equation with fractional derivative and Neumann boundary conditions based on finite element method. The fractional derivative is defined in the Riemann-Liouville sense. The numerical scheme and an example is introduced.

1 Introduction

Fractional calculus is a mathematical discipline which generalizes concept of derivatives and integrals by introducing their non-integer order. Although this field has quite long history (first mentioned by Leibniz in 1695) it attracts attention in last decades. It can be used except of many other fields also for modeling diffusion phenomena. For introduction to the subject [2], [3] can be recommended.

Diffusion is usually simulated by the heat equation $u(x,t)_t = u(x,t)_{xx} + f(x,t)$. However this approach is not suitable for modeling fast diffusion. For that reason the equation is often non-linearly modified. Diffusion can be also modeled by the fractional diffusion equation (FDE), which, in addition, is linear.

In this text we introduce numerical scheme for the fractional diffusion equation using finite element method. Theory of the discrete approximations of the fractional differential equations contains many open questions.

2 Formulation of the problem

We shall deal with initial-boundary value problem with Neumann boundary conditions (flux is prescribed on both ends) in the form

$$
\begin{aligned}
&\frac{\partial}{\partial t}u(x,t) = \frac{\partial^2}{\partial x^2}\,{}_0\mathbf{D}^{-\nu}_{1,x}u(x,t) + f(x,t)\,, \quad x \in (0,1)\,,\ t \in (0,T)\,,\\
&u(x,0) = g(x)\,, \quad x \in (0,1)\,,\\
&\frac{\partial}{\partial x}{}_0\mathbf{D}^{-\nu}_{1,x}u(x,t)\big|_{x=0} = 0\,, \quad t \in (0,T)\,,\\
&\frac{\partial}{\partial x}{}_0\mathbf{D}^{-\nu}_{1,x}u(x,t)\big|_{x=1} = 0\,, \quad t \in (0,T)\,,
\end{aligned}
\tag{1}
$$

where $T > 0$, $f(x,t)$ is a source term and the diffusion term $\frac{\partial^2}{\partial x^2}{}_0\mathbf{D}^{-\nu}_{1,x}u(x,t)$ is an $(2-\nu)$-th order fractional derivative of the function u with respect to the space variable x in the Riemann-Liouville sense for $\nu \in [0,1)$, which will be introduced in details later. Let us remark that if $\nu = 0$ Eq. (1) becomes the classical heat equation.

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For the sake of simplicity the Neumann boundary conditions in the problem (1) are set to zero, adaptation to nonzero ones case causes no problems.

There are several definition of the fractional derivative: Riemann-Liouville, Caputo, Grwünwald-Letnikov and others; more information can be found in [4]. We will work with the Riemann-Liouville approach which is the most common one.

Let $\nu \in \mathbb{R}^+$, $a, b \in \mathbb{R}$ be such that $a < b$, $m \in \mathbb{Z}^+$ be such that $m-1 < \nu < m$ and $\Gamma(\nu)$ be the Gamma function.

The *left fractional integral* of function $f(x)$ is defined by

$$ {}_a\mathbf{D}_x^{-\nu} f(x) = \int_a^x \frac{(x-\xi)^{\nu-1}}{\Gamma(\nu)} f(\xi)\ \mathrm{d}\xi,\ x \in [a, b)\,. $$

The *right fractional integral* is defined by

$$ {}_x\mathbf{D}_b^{-\nu} f(x) = \int_x^b \frac{(x-\xi)^{\nu-1}}{\Gamma(\nu)} f(\xi)\ \mathrm{d}\xi,\ x \in [a, b)\,. $$

Further the *left fractional derivative* is defined by

$$ {}_a\mathbf{D}_x^{\nu} f(x) = \frac{d^m}{dx^m} \int_a^x \frac{(x-\xi)^{\nu-1}}{\Gamma(\nu)} f(\xi)\ \mathrm{d}\xi,\ x \in [a, b)\,, $$

and the *right fractional derivative* is defined by

$$ {}_x\mathbf{D}_b^{\nu} f(x) = \frac{d^m}{dx^m} \int_x^b \frac{(x-\xi)^{\nu-1}}{\Gamma(\nu)} f(\xi)\ \mathrm{d}\xi,\ x \in [a, b)\,. $$

Since we need to consider all points of the interval (a, b), we have to utilize both the left and the right integral. We use also the so-called *Riesz fractional integral* defined by

$$ {}_0\mathbf{D}_1^{-\nu} y(x) = \frac{1}{2}\left({}_0\mathbf{D}_x^{-\nu} y(x) + {}_x\mathbf{D}_1^{-\nu} y(x)\right) = \frac{1}{2}\left(\int_0^x \frac{(x-\xi)^{\nu-1}}{\Gamma(\nu)} y(\xi)\ \mathrm{d}\xi + \int_x^1 \frac{(\xi-x)^{\nu-1}}{\Gamma(\nu)} y(\xi)\ \mathrm{d}\xi\right). $$

3 Discretization of the Fractional Equation

In this section we develop a numerical method for the problem (1). Problems of the numerical solution of FDE are caused by the fact that fractional derivative is not local operator and also by the prescribed Neumann boundary conditions.

The first problem is to decide whether to do discretization first in the time or in the space variable. The fractional derivative is a global operator which is acting, in our case, on the space variable, so during the numerical solution it is necessary to know all values of the space variable in the previous time step(s) and then it is possible to find new ones. Thus to start with the discretization in space variable and then to solve a set of initial ordinary differential problems is not possible. For that reason we perform first the time discretization and then we solve a boundary value problem in each time step. This method is usually called the Rothe method and is described in detail in [5].

Numerical methods of FDE are usually based on the difference fractional calculus, e. g. [1], we shall use another approach based on the finite element method (FEM).

3.1 Time discretization

Let us choose equidistant partition of the interval $(0, T)$ with time step $\tau = T/p$. Approximation of $u(x, k\tau)$ is denoted by $\tilde{u}^k(x)$ and similarly $f^k(x) = f(x, k\tau)$. Time derivative $\frac{\partial}{\partial t}u(x,t)$ is replaced by the difference quotient $\frac{1}{\tau}\left(\tilde{u}^k(x) - \tilde{u}^{k-1}(x)\right)$.

In the weak formulation of time semi-discretized problem we are looking for functions $\tilde{u}^k$ $(k = 1, .., p)$ satisfying $\tilde{u}^0 = g$ and

$$\frac{1}{\tau}\int_0^1 \tilde{u}^k v \,\mathrm{d}x + \int_0^1 \frac{\partial}{\partial x}{}_0\mathbf{D}_1^{-\nu}\tilde{u}^k v' \,\mathrm{d}x = \int_0^1 f^k v \,\mathrm{d}x + \frac{1}{\tau}\int_0^1 \tilde{u}^{k-1} v \,\mathrm{d}x, \tag{2}$$

for all v such that all integrals are properly defined.

3.2 Space discretization

For the sake of simplicity let the space partition of the interval (0,1) be also equidistant with step $h = 1/N$. Let us denote $x_j = jh$, for $j = 0, \dots, N$. Approximation of $\tilde{u}^k(x)$ is denoted by $U^k(x)$ and $U_j^k = U^k(x_j)$. Test functions v are chosen in standard way as piece-wise linear "tent functions".

Let us consider the approximative solution in the form

$$U^k(x) = \sum_{j=0}^{N} U_j^k w_j(x),$$

where w_j are basis functions.

How to choose the set of basis functions? Our choice was influenced by two reasons. First is the fact, that stable solutions of (1) behaves in different way than stable solutions of the heat equation: stable solution of (1) grows near the boundary. We also want the integrals which appear during the derivation of FEM scheme to be analytically computable.

For that reasons inner basis functions w_j $(j = 1, \dots, N-1)$ are piece-wise linear "tent functions" and the boundary basis functions w_0, w_N are chosen in different way, namely

$$w_0(x) = \begin{cases} \dfrac{1}{2NS}\dfrac{1-Nx}{x^{\frac{\nu}{2}}(1-x)^{\frac{\nu}{2}}}, & x \in [0, x_1], \\ 0, & \text{otherwise}, \end{cases} \qquad w_N(x) = \begin{cases} \dfrac{1}{2NS}\dfrac{Nx-N+1}{x^{\frac{\nu}{2}}(1-x)^{\frac{\nu}{2}}}, & x \in [x_{N-1}, 1], \\ 0, & \text{otherwise}, \end{cases}$$

where

$$S = N^{\frac{\nu}{2}-1}\frac{\Gamma(1-\frac{\nu}{2})}{\Gamma(3-\frac{\nu}{2})}\, {}_2F_1\left(\begin{matrix}\frac{\nu}{2}, 1-\frac{\nu}{2} \\ 3-\frac{\nu}{2}\end{matrix}\,\middle|\, \frac{1}{N}\right).$$

The hypergeometric function ${}_2F_1$ is defined by

$${}_2F_1\left(\begin{matrix}a, b \\ c\end{matrix}\,\middle|\, x\right) = \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)}\int_0^1 \frac{t^{b-1}(1-t)^{c-b-1}}{(1-xt)^a}\,\mathrm{d}t = \sum_{k=0}^{\infty}\frac{a^{(k)}b^{(k)}}{c^{(k)}}\frac{x^k}{k!},$$

where $a^{(k)}$ is Pochhammer symbol defined by

$$a^{(k)} = \frac{\Gamma(a+k)}{\Gamma(a)} = \prod_{j=0}^{k-1}(a+j),$$

an example of the set of basis function is on the Figure 1.

Applying all above ideas into (2) yields a system of linear equations for U_j^k. Since the fractional derivative depends on all values in the interval $(0, 1)$ we can not expect that the derivatives of functions w_j $(j = 1, \dots, N-1)$ would be zero outside the interval $[x_{j-1}, x_{j+1}]$.

For that reason the mass matrix of the system is not spare three-diagonal matrix, which usually appears in the finite element solution, but it is a full matrix which has some similar properties as the well-known spare matrix. The elements on the diagonal (except the first and the last one) are positive and in absolute value are larger than the others in its row, elements outside the diagonal are negative and rapidly decreasing to zero. For $\nu = 0$ mass the matrix becomes three-diagonal.

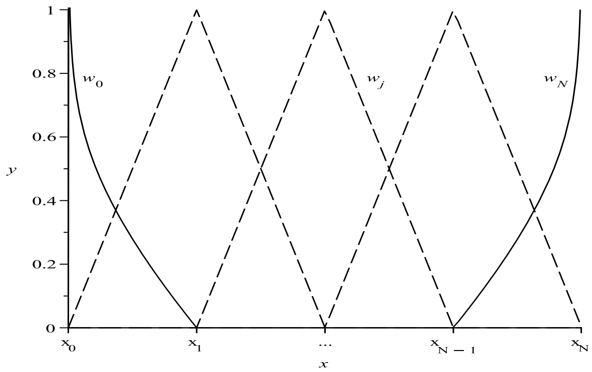

Figure 1. Basis functions for $\nu = 0.8$.

4 Examples

Let us present an example of numerical solution of the problem (1) for the following values of parameters: ν is successively $0, 0.1, 0.3, 0.6$; $T = 0.2$, time step $\tau = 0.01$, space steps $h = 0.02$. The problem is without source term: $f(x,t) \equiv 0$. The initial condition is

$$g(x) = \begin{cases} 2 & \text{for} \quad x \in (0.2; 0.7), \\ 0 & \text{pro} \quad x \notin (0.2; 0.7). \end{cases}$$

The obtained solutions are in Fig. 2. The conservation of mass is evident but there is another interesting effect. With increasing value of ν, the particles are accumulated closer to the boundaries.

5 Conclusion

We developed a numerical scheme which provides numerical solution for initial Neumann boundary value problem involving the Riemann- Liouville fractional differential equations. The key idea is to use Rothe method and FEM with special type of basis functions.

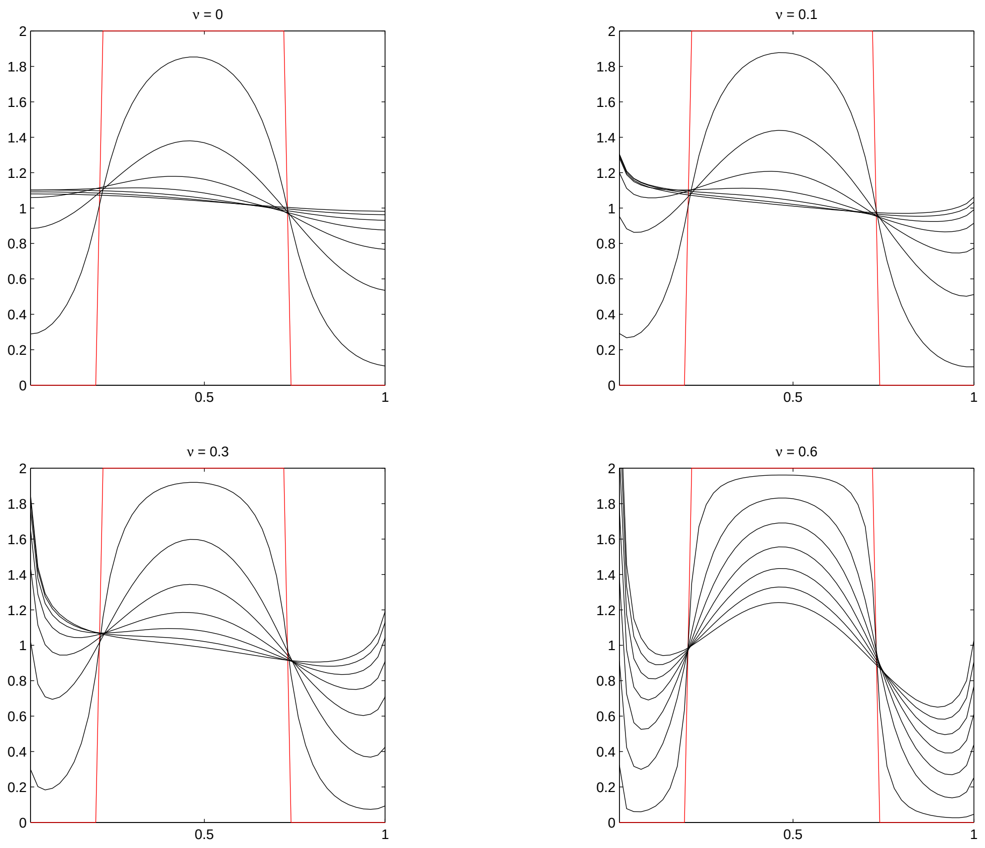

Figure 2. Solutions for the various values of ν

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Authors addresses: *Petra Nováčková*, Institute of Mathematics, Brno University of Technology, Technická 2, CZ-616 69, Brno, Czech Republic, e-mail: `petra.novackova@gmail.com`; *Tomáš Kisela*, Institute of Mathematics, Brno University of Technology, Technická 2, CZ-616 69 Brno, Czech Republic, e-mail: `kisela.tomas@gmail.com`.