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HOW TO SOLVE FRACTIONAL DIFFERENTIAL EQUATIONS DESCRIBING SUBDIFFIUSION IN LAYERED MEDIA*

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We consider subdiffusion in a system which consists of two different media joined together. The media can be separated by a thin partially permeable membrane. Subdiffusion is described by partial differential equations with the time derivative of fractional order. We present the procedure of solving subdiffusion equations for two-layer system. The procedure can be generalized into a multi-layered system.

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Normal and anomalous diffusions are often defined by the time evolution of mean square displacement of a particle $\langle(\Delta x)^2(t)\rangle \sim t^\alpha$. For $0<\alpha<1$ we have subdiffusion, for normal diffusion there is $\alpha = 1$, and when $\alpha > 1$ we have superdiffusion. In the following we consider normal diffusion and subdiffusion processes in a one-dimensional system. Subdiffusion is qualitatively different from normal diffusion. This process occurs in media in which a particle random walk (Brownian motion) is hindered due to their complex

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internal structure. Subdiffusion can occur in porous media, gels, and biological membranes [1–3]. Within the Continuous Time Random Walk model, in subdiffusion medium, the mean waiting time to take particle's next step $\langle\tau\rangle$ is infinite, with heavy-tailed distributions $\omega(t) \sim 1/t^{\alpha+1}$ when $t \mapsto \infty$, whereas for normal diffusion $\langle\tau\rangle$ is finite [4, 5]. Subdiffusive medium is characterized by subdiffusion parameter α and subdiffusion coefficient D. This process is most often described by a partial differential equation with the time derivative of fractional order controlled by α.

Layer media often occur in biological systems. They consist of different layers in which normal diffusion or subdiffusion with different parameters occur. Between the layers, partially permeable thin membranes may be present. In [6–9], boundary conditions at the border between different subdiffusive media have been derived by means of a Particle Random Walk model on a lattice. These conditions involve fractional time derivatives and take different forms depending on initial location of diffusing particles. Therefore, the procedure of solving these equations does not seem to be simple. In this short communication, we present the method of solving fractional subdiffusion equations for a two-layer system. The presented method can be generalized into multi-layer systems. We believe that this method will be helpful in modelling subdiffusion processes in layered systems.

We consider subdiffusion in one-dimensional two-layer system in which thin partially permeable membrane may separate the layers. In the following, the symbol A denotes the region $(-\infty, x_N)$ and the symbol B denotes the region (x_N, ∞), the symbols will be also assigned to the functions and parameters defined in these regions, x_N is the position of the border between media. We denote

$$C(x,t) = \begin{cases} C_A(x,t)\,, & x < x_N\,, \\ C_B(x,t)\,, & x > x_N\,, \end{cases} \tag{1}$$

the initial condition is

$$C(x,0) = \begin{cases} C_{0A}(x)\,, & x < x_N\,, \\ C_{0B}(x)\,, & x > x_N\,. \end{cases} \tag{2}$$

Subdiffusion in the regions A and B is described by the following fractional subdiffusion equations:

$$\frac{\partial C_A(x,t)}{\partial t} = D_A \frac{\partial^{1-\alpha_A}}{\partial t^{1-\alpha_A}} \frac{\partial^2 C_A(x,t)}{\partial x^2}\,, \tag{3}$$

$$\frac{\partial C_B(x,t)}{\partial t} = D_B \frac{\partial^{1-\alpha_B}}{\partial t^{1-\alpha_B}} \frac{\partial^2 C_B(x,t)}{\partial x^2}\,, \tag{4}$$

where $0 < \alpha_A, \alpha_B \leq 1$. The Riemann–Liouville fractional derivative is defined for $0 < \beta < 1$ as

$$\frac{\mathrm{d}^\beta f(t)}{\mathrm{d}t^\beta} = \frac{1}{\Gamma(1-\beta)} \frac{\mathrm{d}}{\mathrm{d}t} \int_0^t \mathrm{d}t' \left(t - t'\right)^{-\beta} f\left(t'\right) .$$

The case of $\alpha_i = 1$ corresponds to the normal diffusion process in the region $i = A, B$; then, the fractional time derivative is absent in the equation.

To solve Eqs. (3) and (4), two boundary conditions (BCs) are assumed at the external walls of the system or at $x = \pm\infty$, but next two BCs should be given at a border between media. One of the boundary conditions shows that the diffusive flux is continuous at the border [6–9]

$$J_A\left(x_N^-, t\right) = J_B\left(x_N^+, t\right) , \tag{5}$$

where

$$J_i(x,t) = -D_i \frac{\partial^{1-\alpha_i}}{\partial t^{1-\alpha_i}} \frac{\partial C_i(x,t)}{\partial x} , \qquad i = A, B . \tag{6}$$

The other boundary condition at the border is different for particles located initially in A and B regions. This fact prompts us to consider separately diffusion of particles located initially in the region A and located initially in the region B. Let us assume that $C_{AA}(x,t)$ and $C_{BA}(x,t)$ are the solutions to Eqs. (3) and (4), respectively, generated by the particles located initially in the region A for which the initial condition is

$$\begin{cases} C_{AA}(x,0) = C_{0A}(x) , & x < x_N , \\ C_{BA}(x,0) = 0 , & x > x_N . \end{cases} \tag{7}$$

Similarly, $C_{AB}(x,t)$ and $C_{BB}(x,t)$ are the solutions to Eqs. (3) and (4) for the initial condition

$$\begin{cases} C_{AB}(x,0) = 0 , & x < x_N , \\ C_{BB}(x,0) = C_{0B}(x) , & x > x_N . \end{cases} \tag{8}$$

The particle concentrations are obtained by means of the formula

$$\begin{cases} C_A(x,t) = C_{AA}(x,t) + C_{AB}(x,t) , & x < x_N , \\ C_B(x,t) = C_{BA}(x,t) + C_{BB}(x,t) , & x > x_N . \end{cases} \tag{9}$$

To solve the subdiffusive equations, we use the Laplace transform $\mathcal{L}[f(t)] = \int_0^\infty \mathrm{e}^{-st} f(t) \mathrm{d}t \equiv \hat{f}(s)$. Due to the formulas $\mathcal{L}\left[\frac{\mathrm{d}f(t)}{\mathrm{d}t}\right] = s\hat{f}(s) - f(0)$ and

$$\mathcal{L}\left[\frac{\mathrm{d}^\beta f(t)}{\mathrm{d}t^\beta}\right] = s^\beta \hat{f}(s) , \qquad 0 < \beta < 1 , \tag{10}$$

in terms of the Laplace transform Eqs. (3) and (4) are

$$s\hat{C}_{Ai}(x,s) - \delta_{Ai}C_{0A}(x) = D_A s^{1-\alpha_A}\frac{\partial^2 \hat{C}_{Ai}(x,s)}{\partial x^2}, \tag{11}$$

$$s\hat{C}_{Bi}(x,s) - \delta_{Bi}C_{0B}(x) = D_B s^{1-\alpha_B}\frac{\partial^2 \hat{C}_{Bi}(x,s)}{\partial x^2}, \tag{12}$$

where δ_{ij} is the Kronecker symbol. The boundary condition (5) reads

$$D_A s^{1-\alpha_A} \left.\frac{\partial \hat{C}_{Ai}(x,s)}{\partial x}\right|_{x=x_N^-} = D_B s^{1-\alpha_B} \left.\frac{\partial \hat{C}_{Bi}(x,s)}{\partial x}\right|_{x=x_N^+}. \tag{13}$$

The second boundary condition is expressed for the functions $\hat{C}_{iA}$ and $\hat{C}_{iB}$ separately. The detailed form of this condition depends on the probabilities of passing a single particle across the border between media. Let us denote by $1-q_A$ the probability of particle passing through the border from the medium A to B and by $1-q_B$ the probability of passing through the border of a particle moving in the opposite direction, see Figs. 1 and 2. The probabilities of particle stopping at the border are q_A and q_B, respectively, $0 \le q_A, q_B \le 1$. We assume that the partially permeable membrane separates the media. Then, we assume that $q_A \neq 0$ and $q_B \neq 0$, this situation is illustrated in Fig. 1. If the boundary between the media is fully permeable

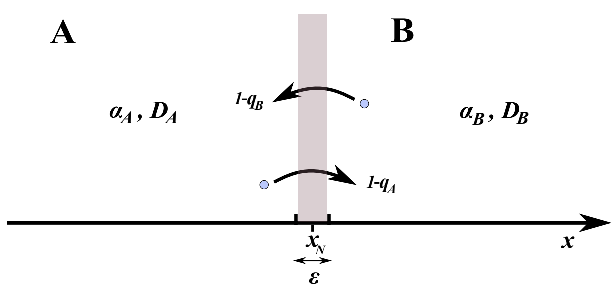

Fig. 1. Diffusion through the membrane that occupies the interval $(x_N - \epsilon/2, x_N + \epsilon/2)$. A particle that tries to get from the region A to B through the membrane can do it with a probability $1-q_A$, and moving in the opposite direction it can pass through the membrane with a probability $1-q_B$, ϵ is the thickness of the membrane.

to particles moving in one direction, which may occur *e.g.* at the porous medium–water border, we have $q_A = 0$ or $q_B = 0$, see Fig. 2. When particles can move freely across the border, we have $q_A = q_B = 0$. In this case, different concentrations of particles at both sides of the border are the result

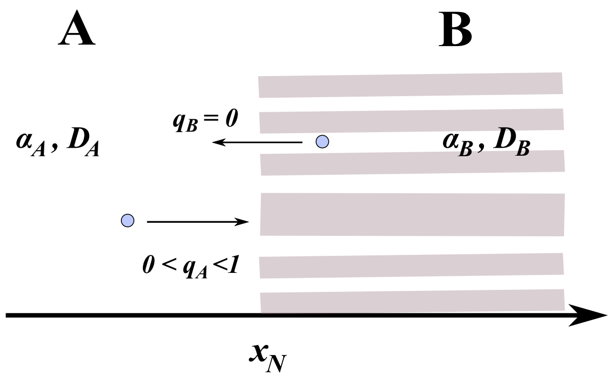

Fig. 2. One-sided fully permeable boundary between media A and B, q_A and q_B are the probabilities of stopping diffusing particle at the border.

of different mobility of the particles in the media. The boundary conditions for the cases mentioned above are qualitatively different. We have [6]

$$\sqrt{D_A} s^{1-\alpha_A/2} \hat{C}_{AA}\left(x_N^-, s\right) = K_A(s) \sqrt{D_B} s^{1-\alpha_B/2} \hat{C}_{BA}\left(x_N^+, s\right) , \tag{14}$$

$$K_B(s) \sqrt{D_A} s^{1-\alpha_A/2} \hat{C}_{AB}\left(x_N^-, s\right) = \sqrt{D_B} s^{1-\alpha_B/2} \hat{C}_{BB}\left(x_N^+, s\right) , \tag{15}$$

where

$$K_A(s) = \begin{cases} \frac{1-q_B}{1-q_A} \sqrt{\frac{D_B}{D_A}} s^{(\alpha_A-\alpha_B)/2} \left(1 + \frac{\epsilon s^{\alpha_B/2}}{(1-q_B)\sqrt{D_B}}\right) , & q_A \neq 0 , \quad q_B \neq 0 , \\ (1-q_B) \sqrt{\frac{D_B}{D_A}} s^{(\alpha_A-\alpha_B)/2} , & q_A = 0 , \quad q_B \neq 0 , \\ \frac{1}{1-q_A} \sqrt{\frac{D_B}{D_A}} s^{(\alpha_A-\alpha_B)/2} , & q_A \neq 0 , \quad q_B = 0 , \\ \sqrt{\frac{D_B}{D_A}} s^{(\alpha_A-\alpha_B)/2} , & q_A = 0 , \quad q_B = 0 , \end{cases} \tag{16}$$

$$K_B(s) = \begin{cases} \frac{1-q_A}{1-q_B} \sqrt{\frac{D_A}{D_B}} s^{(\alpha_B-\alpha_A)/2} \left(1 + \frac{\epsilon s^{\alpha_A/2}}{(1-q_A)\sqrt{D_A}}\right) , & q_A \neq 0 , \quad q_B \neq 0 , \\ \frac{1}{1-q_B} \sqrt{\frac{D_A}{D_B}} s^{(\alpha_B-\alpha_A)/2} , & q_A = 0 , \quad q_B \neq 0 , \\ (1-q_A) \sqrt{\frac{D_A}{D_B}} s^{(\alpha_B-\alpha_A)/2} , & q_A \neq 0 , \quad q_B = 0 , \\ \sqrt{\frac{D_A}{D_B}} s^{(\alpha_B-\alpha_A)/2} , & q_A = 0 , \quad q_B = 0 . \end{cases} \tag{17}$$

Using Eq. (10), it is easy to see that the inverse Laplace transform of Eqs. (14) and (15) provides boundary conditions with fractional time derivatives in the time domain.

Usually, calculation of inverse Laplace transforms for solutions to subdiffusion equations is not easy. However, if the Laplace transform of solution can be present as a series of $\sum_{n=0}^{\infty} a_n s^{\gamma+n\mu} \mathrm{e}^{-b_n s^\beta}$, the inverse Laplace transform can be calculated term by term using the formula [6]

$$\mathcal{L}^{-1}\left[s^\nu \mathrm{e}^{-as^\beta}\right] \equiv f_{\nu,\beta}(t;a) = \frac{1}{t^{\nu+1}} \sum_{k=0}^{\infty} \frac{1}{k!\Gamma(-k\beta-\nu)} \left(-\frac{a}{t^\beta}\right)^k , \tag{18}$$

$a, \beta > 0$; the function $f_{\nu,\beta}$ is a special case of the H-Fox function and the Wright function.

As an example, we present the solutions to Eqs. (3) and (4) for $q_A \neq 0$, $q_B \neq 0$, $0 < \alpha_B < \alpha_A < 1$, and for the initial conditions $C_{0A} = \delta(x - x_0)$, $C_{0B} = 0$, where δ is the delta-Dirac function. In this case, the solution can be interpreted as a probability density $P(x, t; x_0)$ of finding a particle at point x at time t, x_0 is the initial position of the particle at $t = 0$. For $t \gg \max[t_1, t_2]$, where

$$\begin{aligned} t_1 &= (\tilde{\gamma}_B/\Gamma(1-\alpha_B/2))^{2/\alpha_B} , \\ t_2 &= (\tilde{\gamma}_A/\tilde{\gamma}_B \Gamma(1-(\alpha_A-\alpha_B)/2))^{2/(\alpha_A-\alpha_B)} , \end{aligned}$$

and $\tilde{\gamma}_i = \frac{\epsilon}{(1-q_i)\sqrt{D_i}}$, $i = A, B$, we get

$$\begin{aligned} P_A(x,t;x_0) &= \frac{1}{2\sqrt{D_A}} \left[f_{-1+\alpha_A/2,\alpha_A/2}\left(t; \frac{|x-x_0|}{\sqrt{D_A}}\right) \right. \\ &\quad \left. - f_{-1+\alpha_A/2,\alpha_A/2}\left(t; \frac{2x_N - x - x_0}{\sqrt{D_A}}\right) \right] \\ &\quad + \frac{\tilde{\gamma}_A}{\sqrt{D_A}\tilde{\gamma}_B} f_{-1+\alpha_A-\alpha_B/2,\alpha_A/2}\left(t; \frac{2x_N - x - x_0}{\sqrt{D_A}}\right) , \end{aligned} \tag{19}$$

$$\begin{aligned} P_B(x,t;x_0) &= \frac{1}{\sqrt{D_B}} \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{x_0 - x_N}{\sqrt{D_A}}\right)^n \\ &\quad \times \left[f_{-1+\alpha_B/2+n\alpha_A/2,\alpha_B/2}\left(t; \frac{x-x_N}{\sqrt{D_B}}\right) \right. \\ &\quad \left. - \frac{\tilde{\gamma}_A}{\tilde{\gamma}_B} f_{-1+(n+1)\alpha_A/2,\alpha_B/2}\left(t; \frac{x-x_N}{\sqrt{D_B}}\right) \right] . \end{aligned} \tag{20}$$

The solutions to subdiffusion equations in the system presented in Fig. 1, obtained using the method presented in this paper, describe well the process of releasing antibiotics from a gel into water [7]; a coincidence of theoretical functions with experimental data is observed there. The examples of plots of the functions (19) and (20) are presented in Fig. 3.

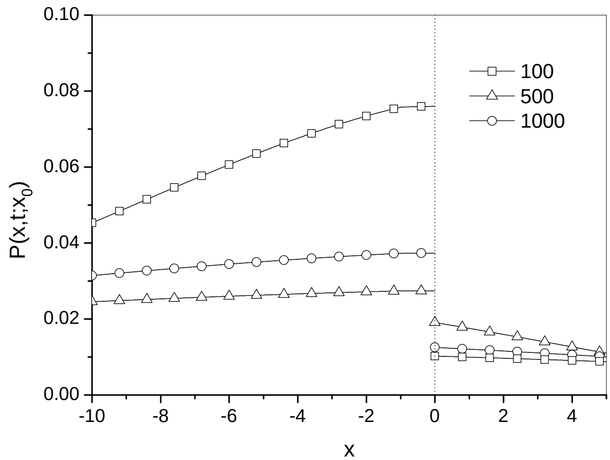

Fig. 3. Plots of the functions (19) and (20) for $\alpha_A = 0.9$, $\alpha_B = 0.6$, $D_A = 1$, $D_B = 2$, $\gamma_A = 0.1$, $\gamma_B = 0.2$, $x_0 = -1$, and $x_N = 0$ for different times given in the legend. All quantities are given in arbitrarily chosen units.

The process of particle diffusion from region $A = (-\infty, x_N)$ to region $B = (x_N, \infty)$ (and *vice versa*) is related to the Sparre–Andersen scaling problem [5, 10]. As part of this problem, the first passage time between the regions is considered. A detailed analysis of this problem for the model considered in this paper will be presented elsewhere. Here we show the distribution of the first passage time between points located in different parts of the system. Let $F_{BA}(x, t; x_0)$ be the probability of arriving for the first time to $x \in B$ at time t, $x_0 \in A$ is the initial particle position. Assuming that $1/2 \leq \alpha_A, \alpha_B \leq 1$, in the limit of long time, we get

$$\begin{aligned} F_{BA}(x,t;x_0) &= a_1 f_{(\alpha_B-\alpha_A)/2,\alpha_A/2}\left(t; \frac{x_N - x_0}{\sqrt{D_A}}\right) \\ &\quad - b_1 f_{\alpha_A-\alpha_B/2,\alpha_A/2}\left(t; \frac{x_N - x_0}{\sqrt{D_A}}\right), \end{aligned} \tag{21}$$

$$\begin{aligned} F_{AB}(x,t;x_0) &= a_2 f_{(\alpha_A-\alpha_B)/2,\alpha_B/2}\left(t; \frac{x_0 - x_N}{\sqrt{D_B}}\right) \\ &\quad - b_2 f_{\alpha_B-\alpha_A/2,\alpha_B/2}\left(t; \frac{x_0 - x_N}{\sqrt{D_B}}\right), \end{aligned} \tag{22}$$

where $a_1 = \sqrt{D_B/D_A}$, $b_1 = (\gamma_A\sqrt{D_B}/D_A)[1+(x-x_N)\gamma_B]$, $a_2 = \sqrt{D_A/D_B}$, and $b_2 = (\gamma_B\sqrt{D_A}/D_B)[1+(x_N-x)\gamma_A]$. In the limit of $t \to \infty$, for $\alpha_A \neq \alpha_B$, we get $F_{BA} \approx c_1/t^{1+(\alpha_A-\alpha_B)/2}$ and $F_{AB} \approx c_2/t^{1+(\alpha_B-\alpha_A)/2}$, where $c_1 = \sqrt{D_B/D_A}/|\Gamma((\alpha_B-\alpha_A)/2)|$, $c_2 = \sqrt{D_A/D_B}/|\Gamma((\alpha_A-\alpha_B)/2)|$. For $\alpha_A = \alpha_B \equiv \alpha$, we obtain $F_{BA} \approx d_1/t^{1+\alpha/2}$ and $F_{AB} \approx d_2/t^{1+\alpha/2}$, where $d_1 = \sqrt{D_B}(x_N-x_0)/(D_A|\Gamma(-\alpha/2)|)$ and $d_2 = \sqrt{D_A}(x_0-x_N)/(D_B|\Gamma(-\alpha/2)|)$. The equations above show that for a sufficiently long time, the function F depends mainly on the difference of subdiffusion parameters α_A and α_B as well as on the region in which the molecule is located at the initial moment. The membrane affects the parameters b_1 and b_2 only and does not affect F within a long-time limit.

We presented the method of solving subdiffusion equations in a two-layer system. Equations (7)–(17) can be generalized to a multi-layer system, so this method can be used to determine the concentration distributions of a diffusing substance in such systems.

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