Схеми Чисельного Інтегрування для Скінченно-Різницевого Розв'язання Дробового за Часом Рівняння Дифузії з Узагальненою Похідною Капуто

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Numerical Integration Schemes for Finite Difference Solution of Time-Fractional Diffusion Equation with Generalized Caputo Derivative

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***Анотація*—У роботі розглядаються алгоритми чисельного обчислення інтегралів, що виникають при дискретизації дробового за часовою змінною рівняння дифузії з узагальненою похідною Капуто. Пропонуються схеми, основані на розкладі підінтегральної функції у ряди Тейлора, що дозволяють пришвидшити обчислення інтегралів порівняно зі схемою рекурсивного підрозбиття. Наводяться результати тестування швидкодії алгоритмів.**

***Abstract*—The algorithms of numerical computation of integrals that arise during the discretization of time-fractional diffusion equation with a generalized Caputo derivative are considered in the paper. We propose several algorithms based on the expansion of the integrand in the Taylor series which allow accelerating the computation of integrals in comparison with the recursive subdivision scheme. The results of the proposed algorithms performance testing are presented.**

Ключові слова—узагальнена похідна Капуто; рівняння дифузії; чисельне інтегрування

Keywords—generalized Caputo derivative; diffusion equation; numerical integration

I. Introduction

Correct mathematical modelling of non-equilibrium diffusion processes requires the use of non-classical differential models, particularly the models with fractional derivatives [1,2]. In the case of media with memory effect, mass transfer is efficiently modelled by introduction of fractional derivative with respect to time variable into the diffusion equation [3,4]. Numerical modelling on the base of such models has higher computational complexity comparing with classical models [5,6]. Generalization of the derivative leads to even higher complexity and makes urgent the development of new numerical algorithms.

The paper deals with numerical modelling of anomalous diffusion using one-dimensional model with generalized Caputo fractional derivative [7] with respect to time variable. Considering the influence of the time spent on computation of integrals arising after discretization of the fractional derivative on the total computation time we propose several specific numerical schemes that lower it.

II. Problem statement and finite difference scheme

We consider the following one-dimensional time-fractional diffusion equation built on the base of the one described in [8]:

$$\sigma D_{t,g}^{(\beta)} C(x,t) = \frac{\partial}{\partial z}\left(d(x,t)\frac{\partial C(x,t)}{\partial z}\right), \quad x \in [0,L],\ t \geq 0,\ \beta \leq 1 \qquad (1)$$

where $C(x,t)$ is the diffusive substance concentration, σ is the porosity of the medium, $d(x,t)$ is the diffusion coefficient, $D_{t,g}^{(\beta)}$ is the generalized Caputo fractional derivative with respect to time variable t that has the following form:

$$D_{t,g}^{(\beta)}H(x,t)=\frac{1}{\Gamma(1-\beta)}\int_0^t\frac{\partial H(x,t)}{\partial t}(g(t)-g(\tau))^{-\beta}d\tau$$

.

For the equation (1) we pose the following initial and boundary conditions:

$$C(0,t)=1,\quad \left.\frac{\partial C(x,t)}{\partial x}\right|_{x=L}=0,\quad C(x,0)=0.$$

Considering uniform grid domain

$$\omega=\left\{(x_i,t_j): x_i=ih, t_j=j\tau,\ i=0,...,m,\ j=0,1,...\right\},\quad (2)$$

first order finite difference approximation $\Delta_{t,g}^{(\beta)}$ of the operator $D_{t,g}^{(\beta)}$ can be defined [7] as

$$\Delta_{t,g}^{(\beta)}C=\frac{1}{\Gamma(1-\beta)}\sum_{s=0}^{j}b_s^{(j)}\frac{C^{s+1}-C^s}{\tau_s},$$

$$b_s^{(j)}=\int_{t_s}^{t_{s+1}}(g(t_j)-g(\tau))^{-\beta}d\tau\quad .\quad (3)$$

Discretizing the equation (1) on the grid (2) using (3) we obtain the following three-diagonal linear equations system (values of C_0^{j+1} and C_m^{j+1} are obtained from the boundary conditions):

$$A_i^jH_{i-1}^{j+1}-R_i^jH_i^{j+1}+B_i^jH_{i+1}^{j+1}=\Omega_i^j\ (i=1,...,m-1,\ j=0,1,...)\quad (4)$$

where

$$A_i^j=\frac{d_{i-1}}{h^2},\quad B_i^j=\frac{d_i}{h^2},\quad R_i^j=\frac{d_{i-1}+d_i}{h^2}+\frac{\sigma b_j^{(j)}}{\tau\Gamma(1-\beta)},$$
$$\Omega_i^j=-\frac{\sigma b_j^{(j)}}{\tau\Gamma(1-\beta)}C^j+\frac{\sigma}{\tau\Gamma(1-\beta)}\sum_{s=0}^{j-1}b_s^{(j)}\left(C^{s+1}-C^s\right).$$

System (4) can be solved by the sweep method [9].

III. Numerical integration algorithms

Determination of the values of system (4) coefficients needs performing calculation of the integrals $b_s^{(j)}$. These integrals are improper when $s=j-1$ and special approximation methods should be used for their evaluation.

We propose to use the following recursive subdivision algorithm for this purpose:

1) The current integration interval $I=[I_l,I_u]$ is set equal to $I=[t_s,t_{s+1}]$;
2) Integral over the current integration interval is calculated using the trapezoidal rule;
3) The interval is then split into two parts: $I_1=[I_l,\frac{1}{2}(I_l+I_u)]$ and $I_2=[\frac{1}{2}(I_l+I_u),I_u]$. The value of the integral over the interval $I=[I_l,I_u]$ is calculated as a sum of integrals over the intervals I_1, I_2, that are, in turn, evaluated using the trapezoidal rule;
4) When the difference between the approximations of the integral's value obtained on steps 2 and 3 is greater than a given ε_1, the procedure is recursively repeated for the intervals I_1, I_2.

When $s=j-1$ and the integral has to be computed over the interval $I_3=[t_{s+1}-\varepsilon_2,t_{s+1}]$ where ε_2 is a given constant, we propose to use the following algorithm:

1) The initial step is set equal to $s=\varepsilon_2/N$ where N is a given number; the initial value of the lower bound of integration interval is set equal to $t_l=t_{s+1}-\varepsilon_2$.
2) The value of the integral over $[t_l,t_l+s]$ is calculated by a 4-th order quadrature formula;
3) When $F(t_l+s/2)/F(t_l)<F(t_l+s)/F(t_l+s/2)$ where F is an integrand, we decrease the step s by $F(t_l+s)F(t_l)/F^2(t_l+s/2)$. This makes the integrand to be close to a linear function within the interval $[t_l,t_l+s]$;
4) The step is halved when $t_l+s>t_{s+1}$;
5) When $(t_{s+1}-t_l)<\varepsilon_3$ where ε_3 is a given constant, we shift to the next interval by setting $t_l\leftarrow t_l+s$.

Number of evaluations upon the above-described algorithm that must be performed increases with an increase of time step number. Since it is difficult to construct optimized or recurrent procedures for this algorithm, the construction of other numerical schemes is urgent in order to reduce the time spent on computing the integrals $b_s^{(j)}$.

Assuming there exists an infinitely differentiated function $f(\tau): f(g(\tau))=\tau$, the integral $b_s^{(j)}$ can be expanded in series in two following ways.

After doing in $b_s^{(j)}$ a change of variables in the form of $x=g(t_j)-g(\tau)\Rightarrow\tau=f(g(t_j)-x)$ we obtain

$$b_s^{(j)}=\int_{t_s}^{t_{s+1}}(g(t_j)-g(\tau))^{-\beta}d\tau=\int_{g(t_j)-g(t_{s+1})}^{g(t_j)-g(t_s)}f'(g(t_j)-x)x^{-\beta}dx.$$

Expanding $f'(x)$ in the Taylor series at $x=g(t_j)$ we have

$$b_s^{(j)} = \sum_{n=0}^{\infty}\left((-1)^n \frac{f^{(n+1)}(g(t_j))}{n!} \int_{g(t_j)-g(t_{s+1})}^{g(t_j)-g(t_s)} x^{n-\beta} dx \right) =$$

$$= \sum_{n=0}^{\infty}\left((-1)^n \frac{f^{(n+1)}(g(t_j))}{n!(n-\beta+1)} \left[\begin{matrix} (g(t_j)-g(t_s))^{n-\beta+1} \\ -(g(t_j)-g(t_{s+1}))^{n-\beta+1} \end{matrix} \right] \right). \quad (5)$$

Another scheme of $b_s^{(j)}$ evaluation can be obtained doing a change of variables in the form of $x = g(\tau) \Rightarrow \tau = f(x)$ having

$$b_s^{(j)} = \int_{t_s}^{t_{s+1}} (g(t_j)-g(\tau))^{-\beta} d\tau = \int_{g(t_s)}^{g(t_{s+1})} f'(x)(g(t_j)-x)^{-\beta} dx.$$

Expanding $(g(t_j)-x)^{-\beta}$ using the generalized Newton binomial series and expanding $f'(x)$ in the Taylor series at $x = g(t_{s+1})$ we have

$$b_s^{(j)} = \sum_{n=0}^{\infty}\left((-1)^n \binom{-\beta}{n} g(t_j)^{-\beta-n} S_n \right),$$

$$S_n(t_s, t_{s+1}) = \sum_{m=0}^{\infty}\left[B_m \frac{f^{(m+1)}(g(t_{s+1}))}{m!} \right],$$

$$B_m = \int_{g(t_s)}^{g(t_{s+1})} x^n (x - g(t_{s+1}))^m dx. \quad (6)$$

The value of the integral B_1 can be calculated using the following recursion:

$$B_0 = \int_{g(t_s)}^{g(t_{s+1})} x^n dx = \frac{1}{n+1}(g(t_{s+1})^{n+1} - g(t_s)^{n+1}),$$

$$B_{i+1} = -\frac{n+i+2}{g(t_{s+1})(i+1)}\left(B_i - \frac{g(t_s)^{n+1}(g(t_s)-g(t_{s+1}))^{i+1}}{g(t_{s+1})(i+1)} \right).$$

The main feature of the scheme (6) is that the values of the coefficients S_n once calculated for the fixed t_s and t_{s+1} can be cached and further used when t_j changes.

Computational experiments performed in the case of $g(\tau) = \tau^2$, $f(\tau) = \tau^{1/2}$, $f'(\tau) = \frac{1}{2}\tau^{-1/2}$, $f^{(n+1)}(\tau) = \frac{1/2-n}{\tau} f^{(n)}(\tau)$ showed that the convergence of the series (5) worsens when $t_s \to 0$ while the convergence of the series (6) worsens when $t_{s+1} \to t_j$. To ensure the highest performance we propose the following algorithm of automatic selection of series (5) or (6) for the approximation of the integrals $b_s^{(j)}$ depending on the values of their parameters:

1) Let the values of the integrals $b_s^{(j)}$ are calculated sequentially for t_j, $j = 0,1,...$ and t_s, $s = 0,...,j-1$;
2) $a \leftarrow 2$;
3) When $t_s \le t_a$, the scheme (6) is used for numerical integration;
4) When $t_s = t_a$ we perform a correction of the value of the parameter a. If the number of iterations needed to approximate the integral with a given accuracy using the scheme (5) is greater that the corresponding number of iterations for the scheme (6), the value of the parameter must be increased: $a \leftarrow a+1$. Otherwise, if $a \ne 1$ the value must be set to $a \leftarrow a-1$;
5) When $t_s > t_a$, the scheme (5) is used for numerical integration.

IV. Numerical experiments

The efficiency of the proposed algorithms was tested solving the initial-boundary problem for the equation (1) with $L = 3$, $d = 1$, $\sigma = 1$, $\beta = 0.6$, $\tau = 0.1$. The obtained solutions are presented for $T = 5$ on Fig. 1.

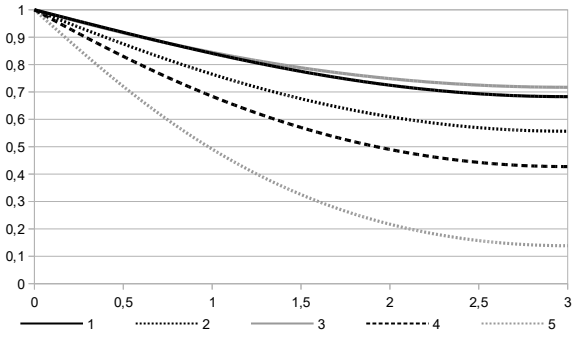

Fig. 1. Solutions of the initial-boundary problem for the equation (1) (1 - $\beta = 1$, 2 - $\beta = 0.8$, $g(\tau) = \tau$, 3 - $\beta = 0.6$, $g(\tau) = \tau^2$, 4 - $\beta = 0.6$, $g(\tau) = \tau$, 5 - $\beta = 0.8$, $g(\tau) = \tau^{1/2}$)

Total time (ms) spent during the solution of the problem on the calculations of $b_s^{(j)}$ for $g(\tau) = \tau^2$ depending on the number of time step is given on Fig.2.

As can be seen from the experimental data, the algorithm for automatic selection of series (5) or (6) allows accelerating the calculation, whereas the use of these series separately due to the peculiarities of their convergence slows down the solution process.

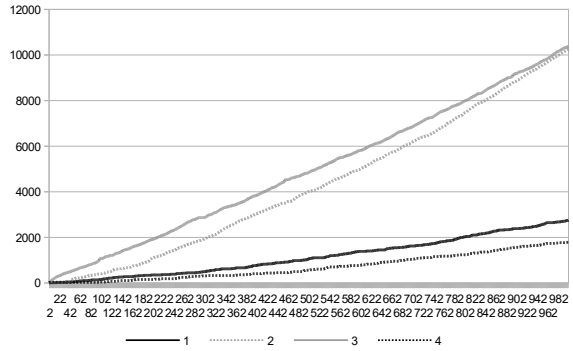

Fig. 2. Time spent to compute the value of $b_s^{(j)}$ depending on the number of time step (1 – the recursive subdivision algorithm, 2 – the series (5), 3 – the series (6), 4 – the algorithm of automatic series selection)

Computational experiments showed that the efficiency of the algorithm of automatic series selection decreases with the increase of time step number. At the same time, it increases with the decrease of the fractional derivative order β or the increase of time step length.

The per cent of the time spent on the calculations of $b_s^{(j)}$ in the total time depending on the number of time step is shown on Fig.3. The obtained data show that the influence of the time spent on computing $b_s^{(j)}$ on the total time decreases with the increase of the number of time step.

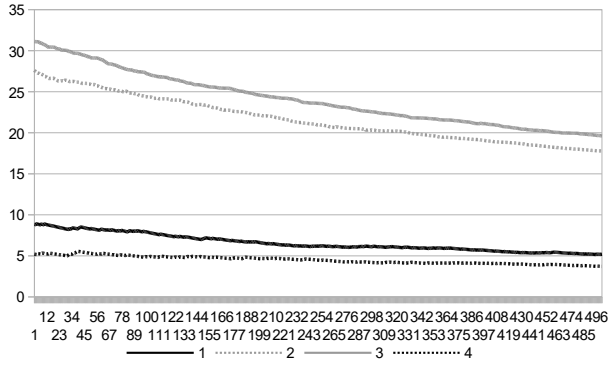

Fig. 3. Per cent of the time spent on the calculations of $b_s^{(j)}$ in the total time depending on the number of time step (1 – the recursive subdivision algorithm, 2 – the series (5), 3 – the series (6), 4 – the algorithm of automatic series selection)

CONCLUSIONS

Improper integrals that arise in discretization of generalized Caputo derivative have to be numerically calculated during modelling of anomalous diffusion on the base of the considered model. As recursive subdivision quadrature formulae that can be used in this case are rather slow, we propose specific computation schemes that can speed-up computations.

The performed computational experiments show that the use of the schemes based of Taylor series expansions of the integrals $b_s^{(j)}$ can achieve up to 2.5 times speed-up solving the considered problem of diffusion process simulation. The speed-up lowers here while modelling the processes on large time intervals; become higher for lower values of time step or higher values of fractional derivative order.

As the proposed algorithms are optimized for the case of sequential changes of the parameters of the integrals $b_s^{(j)}$, further research can be performed to apply them for solving space-fractional differential equation with generalized Caputo derivatives.

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