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Numerical Solution of a Nonlinear Fractional Diffusion Problem

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Abstract:

This article constructs a numerical solution for a nonlinear diffusion equation with a time-fractional derivative. The considered problem is posed on a semi-infinite domain, where the diffusion coefficient is expressed through a power function of the solution. The boundary condition of the problem also has a nonlinear form. The time-fractional derivative is discretized by an L1-type fractional difference approximation, while the spatial operator is discretized by the finite difference method in conservative form. The nonlinear diffusion coefficient is taken from the previous time layer, leading to a semi-implicit scheme. As a result, a tridiagonal system of linear algebraic equations is obtained at each time layer. This approach simplifies the computational process, improves stability, and provides a convenient framework for practical implementation.

Keywords: *fractional derivative, Caputo derivative, L1 scheme, nonlinear diffusion, finite difference method, semi-implicit scheme, numerical solution.*

Introduction

Fractional differential equations play an important role in the mathematical modeling of processes with memory effects. In classical differential equations, the current state of a process mainly depends on the current time and spatial variables, whereas in fractional-order equations the states at previous time layers are also taken into account. Therefore, such equations are used to describe anomalous diffusion, filtration, heat transfer, biological population dynamics, and mass transfer processes in complex media. [1-5, 7]

This paper considers the following nonlinear fractional diffusion problem:

$$\frac{\partial}{\partial x}\left(u^m \frac{\partial u}{\partial x}\right), \qquad x \in R_+, \quad t > 0,$$
$$-u^q(0,t),$$
$$u(x,0) = u_0(x), \qquad x \in R_+.$$

Here, $(0<\alpha<1)$, $(m>0)$, $(q>0)$, $(u\_0(x))$ is considered as a compactly supported nonnegative initial function.

The main purpose of the article is to construct a semi-implicit numerical scheme for solving this problem based on an L1-type fractional difference scheme and the finite difference method with respect to the spatial variable. [8-11, 13, 14]

2. Mathematical formulation of the problem

The considered problem is written as follows:

$$\frac{\partial}{\partial x}\left(u^m(x,t)\frac{\partial u(x,t)}{\partial x}\right), \qquad x>0, \quad t>0.$$

Here, $({}^C D_t^\alpha u)$ is the fractional derivative in the Caputo sense, defined as follows: [6]

$$\frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{\partial u(x,s)}{\partial s}\frac{ds}{(t-s)^\alpha}, \qquad 0<\alpha<1.$$

The following nonlinear boundary condition is given at the left boundary:

$$u^m(0,t)u_x(0,t) = -u^q(0,t).$$

The initial condition is:

$$u(x,0) = u\_0(x).$$

In practical numerical computations, the semi-infinite domain is replaced by a finite interval:

$$0 \le x \le L.$$

Here, (L) is chosen sufficiently large. If the initial function is compactly supported, the value of the solution near $(x=L)$ is sufficiently small. Therefore, the following condition is imposed at the right boundary: [15]

$$u(L,t) = 0.$$

3. Construction of the difference grid

A uniform grid is introduced on the computational domain as follows:

$$x_i = ih, \qquad i = 0,1,\dots,N,$$
$$t_n = n\tau, \qquad n = 0,1,\dots,M.$$

where

$$h = \frac{L}{N}, \qquad \tau = \frac{T}{M}.$$

The numerical solution is denoted as follows:

$$u_i^n \approx u(x_i, t_n).$$

The objective is to determine the (u_i^n) values successively over the time layers.

4. L1-type fractional difference approximation in time

The Caputo derivative at (t_{n+1}) is approximated by the L1-type fractional difference scheme as follows: [8-11]

$$^{C}D_t^{\alpha}u(x_i,t_{n+1}) \approx \frac{1}{\tau^{\alpha}\Gamma(2-\alpha)}\sum_{k=0}^{n} a_k\left(u_i^{n+1-k}-u_i^{n-k}\right),$$

where

$$a_k=(k+1)^{1-\alpha}-k^{1-\alpha}, \qquad k=0,1,\ldots,n.$$

Introduce the following notation:

$$\mu=\tau^{\alpha}\Gamma(2-\alpha).$$

Then the L1 approximation can be written in the following form:

$$^{C}D_t^{\alpha}u(x_i,t_{n+1}) \approx \frac{1}{\mu}\left[u_i^{n+1}-u_i^{n}+\sum_{k=1}^{n} a_k\left(u_i^{n+1-k}-u_i^{n-k}\right)\right].$$

This expression takes into account the memory property of the fractional derivative. That is, the solution at the new time layer is related to the values at the previous time layers. [8-11]

5. Approximation of the spatial operator by finite differences

The nonlinear diffusion operator on the right-hand side of the equation is given in conservative form:

$$\frac{\partial}{\partial x}\left(u^{m}\frac{\partial u}{\partial x}\right).$$

We approximate this operator by finite differences as follows: [13, 16]

$$A^{n}_{i-\frac{1}{2}}\frac{u_i^{n+1}-u_{i-1}^{n+1}}{h}n$$

Here, the diffusion coefficients are taken from the previous time layer:

$$\left(\frac{u_i^{n}+u_{i+1}^{n}}{2}\right)^{m},\ \left(\frac{u_{i-1}^{n}+u_i^{n}}{2}\right)^{m}.$$

Taking the coefficients at the (n)-th layer makes the scheme semi-implicit. That is, the nonlinear diffusion coefficient is taken as a known value from the previous layer, while the unknown (u_i^{n+1}) values are involved at the new layer. As a result, a system of linear algebraic equations is obtained at each time layer. [14, 16]

6. Semi-implicit numerical scheme

Combining the L1-type fractional difference scheme and the spatial finite difference approximation, the following semi-implicit numerical scheme is obtained: [8-11, 13, 14]

$$A^{n}_{i-\frac{1}{2}}\left(u_i^{n+1}-u_{i-1}^{n+1}\right)n$$

This equation is written for the $(i=1,2,\ldots,N-1)$ internal nodes.

We transform the equation into algebraic form:

$$rA^{n}_{i+\frac{1}{2}}u_{i+1}^{n+1}F_i^{n},$$

where

$$r=\frac{\mu}{h^{2}},$$

$$u_i^{n}\sum_{k=1}^{n} a_k\left(u_i^{n+1-k}-u_i^{n-k}\right)$$

Thus, at each time layer, the following tridiagonal system of linear algebraic equations is obtained: F_i^n.

Here

$$\alpha_i = -rA^n_{i-\frac{1}{2}},$$

$$\beta_i = 1 + r\left(A^n_{i-\frac{1}{2}} + A^n_{i+\frac{1}{2}}\right),$$

$$\gamma_i = -rA^n_{i+\frac{1}{2}}.$$

Since the resulting system is tridiagonal, it can be solved efficiently by the Thomas algorithm. [13, 16]

7. Discretization of boundary conditions

The following nonlinear condition is given at the left boundary:

$$u^m(0,t)u_x(0,t) = -u^q(0,t).$$

We write it using a finite difference as follows: $-(u_0^n)^q$.

Here, the (u^m) and (u^q) terms are taken from the previous time layer. As a result, the boundary condition also has a semi-implicit form: [14]

$$-h(u_0^n)^{q-m}.$$

Hence

$$u_1^{n+1} + h(u_0^n)^{q-m}$$

is obtained.

If $(q < m)$ and $(u_0^n = 0)$ occurs, then to avoid division by zero or the appearance of very large values in numerical computations, a small $(\varepsilon > 0)$ regularization can be introduced: [14, 15]

$$(u_0^n)^{q-m} \approx (u_0^n + \varepsilon)^{q-m}.$$

At the right boundary, the following condition is imposed:

$$u_N^{n+1} = 0.$$

8. Computational algorithm

Based on the above scheme, the computational algorithm is constructed as follows.

1. Initial parameters are chosen:

$$\alpha, \quad m, \quad q, \quad L, \quad T, \quad N, \quad M.$$

2. The grid steps are determined:

$$h = \frac{L}{N}, \qquad \tau = \frac{T}{M}.$$

3. Initial values are prescribed:

$$u_i^0 = u_0(x_i), \qquad i = 0,1,\dots,N.$$

4. The coefficients of the L1 scheme are calculated:

$$a_k = (k+1)^{1-\alpha} - k^{1-\alpha}.$$

5. At each $(n = 0,1,\dots,M-1)$ time layer, the diffusion coefficients are determined:

$$\left(\frac{u_i^n + u_{i+1}^n}{2}\right)^m.$$

6. The right-hand side terms are calculated:

$$u_i^n \sum_{k=1}^{n} a_k \left(u_i^{n+1-k} - u_i^{n-k}\right).$$

7. A tridiagonal system of linear algebraic equations is constructed. [13, 16]
8. Boundary conditions are taken into account:

$$u_1^{n+1} + h(u_0^n)^{q-m}, \qquad u_N^{n+1} = 0.$$

9. The resulting system is solved by the Thomas algorithm. [13, 16]
10. The results are stored in the form (u_i^{n+1}) and the computation proceeds to the next time layer.

9. Solution by the Thomas algorithm

From the semi-implicit scheme, at each time layer $(u_i^{n+1}), (i = 1, 2, \ldots, N-1)$, a tridiagonal system of linear algebraic equations is obtained with respect to the unknowns. [13, 16]

The scheme obtained for the internal nodes was as follows:

$$rA^n_{i+\frac{1}{2}} u_{i+1}^{n+1}$$

$$F_i^n$$

where

$$r = \frac{\mu}{h^2}, \qquad \mu = \tau^{\alpha}\Gamma(2-\alpha),$$

$$u_i^n \sum_{k=1}^{n} a_k \left(u_i^{n+1-k} - u_i^{n-k}\right).$$

From the left boundary condition,

$$u_1^{n+1} + h(u_0^n)^{q-m}$$

the following relation is obtained. Therefore, for $(i = 1)$ in the equation, the above expression is substituted for (u_0^{n+1}):

$$rA^n_{\frac{3}{2}} u_2^{n+1} F_1^n.$$

Substituting

$$u_1^{n+1} + h(u_0^n)^{q-m}$$

we obtain the first equation in the following form:

$$rA^n_{\frac{3}{2}} u_2^{n+1} F_1^n + rhA^n_{\frac{1}{2}} (u_0^n)^{q-m}.$$

For the internal nodes $(i = 2, 3, \ldots, N-2)$, the tridiagonal equations are written as follows:

$$rA^n_{i+\frac{1}{2}} u_{i+1}^{n+1} F_i^n.$$

At the right boundary,

$$u_N^{n+1} = 0$$

since this condition holds, for $(i = N-1)$ the following equation is obtained:

$$F_{N-1}^{n}.$$

Thus, for the unknown vector $(U^{n+1}=(u_1^{n+1},u_2^{n+1},\ldots,u_{N-1}^{n+1})^T)$ the following tridiagonal system is obtained:

$$d_1u_1^{n+1}+c_1u_2^{n+1}=\varphi_1,$$

$$\varphi_i,\qquad i=2,3,\ldots,N-2,$$

$$\varphi_{N-1}.$$

Here, the coefficients are defined as follows:

$$d_1=1+rA_{\frac{3}{2}}^{n},\qquad c_1=-rA_{\frac{3}{2}}^{n},$$

$$F_1^n+rhA_{\frac{1}{2}}^{n}(u_0^n)^{q-m},$$

$$a_i=-rA_{i-\frac{1}{2}}^{n},\qquad d_i=1+r\left(A_{i-\frac{1}{2}}^{n}+A_{i+\frac{1}{2}}^{n}\right),\qquad c_i=-rA_{i+\frac{1}{2}}^{n},$$

$$\varphi_i=F_i^n,\qquad i=2,3,\ldots,N-2,$$

$$a_{N-1}=-rA_{N-\frac{3}{2}}^{n},$$

$$1+r\left(A_{N-\frac{3}{2}}^{n}+A_{N-\frac{1}{2}}^{n}\right),$$

$$\varphi_{N-1}=F_{N-1}^{n}.$$

Thus, at each time layer, the posed fractional nonlinear diffusion problem is reduced to the following tridiagonal system in matrix form:

$$\left(\varphi_1,\varphi_2,\varphi_3,...,\varphi_{N-1}\right).$$

Since the resulting system is tridiagonal, it can be solved efficiently by the Thomas algorithm. [13, 16]

In the Thomas algorithm, first the forward sweep is performed. At the first step,

$$P_1=-\frac{c_1}{d_1},\qquad Q_1=\frac{\varphi_1}{d_1}$$

are determined. For the subsequent $(i=2,3,\ldots,N-1)$ values

$$P_i=-\frac{c_i}{d_i+a_iP_{i-1}},$$

$$Q_i=\frac{\varphi_i-a_iQ_{i-1}}{d_i+a_iP_{i-1}}$$

are used for computation.

Then the backward substitution is performed. First,

$$u_{N-1}^{n+1}=Q_{N-1}$$

is taken, and then

$$P_iu_{i+1}^{n+1}+Q_i,\qquad i=N-2,N-3,\ldots,1,$$

is used to determine the remaining unknowns.

After that, the value at the left boundary

$$u_1^{n+1} + h(u_0^n)^{q-m}$$

is recovered by this formula, while at the right boundary

$$u_N^{n+1} = 0$$

is taken.

The computational complexity of the Thomas algorithm is $\left(O\left(N\right)\right)$; therefore, this method is also convenient for large-scale discrete grids. [13, 16]

10. Advantages of the semi-implicit scheme

The proposed semi-implicit scheme has several important advantages.

First, the L1-type fractional difference scheme in time takes into account the memory property of the fractional derivative. [8-11]

Second, the spatial operator is approximated in conservative form. [13, 16]

Third, since the nonlinear diffusion coefficient is taken from the previous time layer, a system of linear algebraic equations is obtained at each time layer.

Fourth, because the resulting linear system is tridiagonal, it can be solved quickly and efficiently by the Thomas algorithm. [13, 16]

Fifth, compared with fully explicit schemes, the semi-implicit scheme has better stability properties. [3, 13, 14]

11. Sample initial function for a numerical experiment

The following compactly supported initial function may be used for numerical experiments:

$$u_0(x) = \left\{(1-x^2)^2, \quad 0 \le x \le 1 \quad .\right\}$$

For example, the following parameters can be chosen:

$$\alpha = 0.5, \qquad m = 2, \qquad q = 1,$$

$$L = 5, \qquad T = 1, \qquad N = 100, \qquad M = 200.$$

In this case, the grid steps are as follows:

$$h = 0.05, \qquad \tau = 0.005.$$

As a result of the numerical computations, the time evolution of the $\left(u\left(x,t\right)\right)$ function, the displacement of the diffusion front, and the influence of the nonlinear flux at the boundary are analyzed. A decrease in the (α) parameter slows down the process, since the fractional derivative strengthens the memory effect. An increase in the $\left(m\right)$ parameter strengthens the dependence of the diffusion coefficient on the solution value. The $\left(q\right)$ parameter determines the absorption or flux intensity at the $\left(x=0\right)$ boundary. [8-11, 15]

12. Error and convergence order

For smooth solutions, the order of approximation of the L1-type scheme in time is usually estimated as follows: $O(\tau^{2-\alpha})$. [8-11]

Since the spatial finite difference approximation is constructed on the basis of central differences, it has the following accuracy: $O(h^2)$.

Therefore, the total error estimate can be expressed as follows: [13, 16]

$$|u(x_i,t_n) - u_i^n| \le C\left(\tau^{2-\alpha} + h^2\right),$$

where $\left(C\right)$ is a positive constant independent of the grid steps.

13. Conclusion

The considered problem describes a nonlinear diffusion process. The presence of the (u^m) coefficient in the equation means that the diffusion rate depends on the solution itself. If (u) is small, diffusion slows down; if (u) is large, diffusion accelerates. Such a property occurs in filtration, heat transfer, and biological population dynamics. [15]

The time-fractional derivative means that the process has memory. In other words, the current state of the system depends not only on the current time but also on its previous states. The L1-type fractional difference scheme naturally represents this memory effect through a discrete sum. [1-4, 8-11]

In the semi-implicit scheme, nonlinear terms are taken from the previous time layer. This significantly simplifies the computations. In a fully implicit scheme, a nonlinear algebraic system is obtained at each time layer, and it must be solved by Newton's method or other iterative methods. In the semi-implicit approach, however, a linear algebraic system is obtained, which is convenient from the viewpoint of programming and computation. [14, 16]

In this article, a semi-implicit numerical scheme based on the L1-type fractional difference scheme and the finite difference method was constructed for a nonlinear fractional diffusion equation. The time-fractional Caputo derivative was discretized by the L1 approximation, while the spatial nonlinear diffusion operator was discretized by conservative finite differences. Since the nonlinear coefficients were taken from the previous time layer, a tridiagonal system of linear algebraic equations was obtained at each time layer. [8-11, 13, 14]

The proposed semi-implicit scheme is computationally simple, stable, and convenient for practical problems. This approach can be used for the numerical modeling of fractional diffusion, anomalous transport, filtration, and heat transfer processes. [1, 2, 14, 15]

In future work, it is advisable to conduct numerical experiments for various (α), (m) and (q) parameters, analyze the results graphically, and study the stability and convergence properties of the scheme in greater depth.

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