A numerical method for solving the time fractional reaction-diffusion equation with variable coefficients on the whole line

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Abstract. This paper focuses on numerically solving the time fractional reaction-diffusion equation on the whole line. A numerical scheme is constructed based on Hermite pseudospectral method, we use finite difference scheme in time direction while Hermite-Gauss points in space. Several numerical results for the Hermite pseudospectral scheme are provided to confirm that a second-order time accuracy and spectral accuracy in space can be obtained.

1. Introduction
In recent years, fractional partial differential equations (FPDEs) have drawn much attention to many scientists to study them both in theoretically and numerically. FPDEs provide a significant tool and they are very popular in describing a variety of physical phenomena, biological systems, chemical processes, economical products and other sciences [1,2].

Time fractional reaction-diffusion equation is one of the most important FPDEs, which has received much attention in recent years, many papers are mainly concern this equation with constant coefficients in bounded domain, while for the equation with variable coefficients in unbounded area, there are few papers in the literature. As is known to all, it is hard to solve this equation with variable coefficients theoretically, then numerical method is a choice to deal with this kind of problem. This gives us a motivation to numerically study the following time fractional reaction-diffusion equation with two variable coefficients on the whole line:

$$\begin{align*}
\frac{cD_{0,t}^{\alpha}}{\Gamma(1-\alpha)} u(x,t) - c x b(x,t) \frac{\partial u(x,t)}{\partial x} + c c(x,t) u(x,t) &= f(x,t), \quad 0 < t \leq T, \\
u(x,0) &= u(x), \quad x \in \mathbb{R}, \\
\lim_{|x| \to \infty} \frac{\partial u(x,t)}{\partial x} &= 0, \quad 0 < t \leq T.
\end{align*}$$

(1.1)

(1.2)

(1.3)

Where \(\alpha (0 < \alpha < 1)\) is the time fractional order which is in the sense of Caputo derivative, \(b(x,t) \geq c_0 > 0, \ c(x,t) \geq c_1 > 0\) and \(f(x,t)\) are all smooth functions. When \(\alpha = 1\), (1.1) represents the classical diffusion equation. The definition of Caputo fractional derivative is:

$$\frac{cD_{0,t}^{\alpha}}{\Gamma(1-\alpha)} u(x,t) = \frac{1}{\Gamma(1-\alpha)} \int_{0}^{t} \frac{\partial s u(x,s)}{(t-s)^{\alpha}} \ ds,$$

for more details about Caputo fractional derivative, readers can refer to [3].

Caputo fractional derivative with order \(0 < \alpha < 1\) is usually discretized in the form of L1-approximation, the convergence order is \(O(t^{2-\alpha})\). Readers can refer to some high order approximation schemes of Caputo fractional derivative, see [4]. We will take the advantage of the \(L2 - 1_{\sigma}\) formula which is proposed in [4], then we can obtain the second order in time accuracy.
In this paper, we numerically solve the time fractional reaction-diffusion equation (1.1)-(1.3) by using Hermite pseudospectral method with Hermite-Gauss points in space, as far as we know there are only a few papers studying Hermite spectral method for solving FPDEs, interested readers can refer to [5] and references therein.

This paper is organized as follows. In section 2, several important preliminaries about Hermite functions and interpolation is introduced. The $L2-1_{\alpha}$ formula is used in discretizing the Caputo fractional derivative, then a fully discrete Hermite pseudospectral scheme is proposed in section 3. In section 4, we do several numerical experiments to test the efficiency of our scheme.

2. Preliminaries and notations
In this section, we mainly introduce some important properties of Hermite functions and its relative definitions. The Hermite functions are given by

$$H_l(x) = \frac{1}{\sqrt{\pi}} e^{-\frac{x^2}{2}} H_l(x), \quad l = 0, 1, 2, \cdots,$$

where $H_l$ denotes the Hermite polynomial with degree $l$. The orthogonal relation is

$$\int_{-\infty}^{\infty} H_l(x) H_m(x) dx = \delta_{l,m},$$

where $\delta_{l,m}$ is the Kronecker function. For more detail about Hermite functions, see the reference [6].

For any function $v$, we can write it in the form $v = \sum_{l=0}^{\infty} \hat{v}_l H_l(x)$, where

$$\hat{v}_l = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} v(x) H_l(x) dx, \quad l = 0, 1, 2, \cdots,$$

where $\hat{v}_l$ are the Hermite coefficients. For any given positive integer $N$, define

$$P_N = \text{span}\{H_0(x), H_1(x), \cdots, H_N(x)\}.$$

Set $\{x_j\}_{j=0}^{N}$ be the zeros of $H_{N+1}$, and $\{w_j\}_{j=0}^{N}$ are modified Hermite-Gauss weight, see [6], that is

$$w_j = \frac{1}{(N+1) \hat{H}_N^2(x_j)}.$$

Let $(u, v)_N$ denote the discrete inner product and $||v||_N$ represent the corresponding discrete norm, the definitions are given by

$$(u, v)_N = \sum_{j=0}^{N} u(x_j) v(x_j) w_j, \quad ||v||_N = (u, v)_{N}^{\frac{1}{2}}.$$

For any $\varphi \in P_m, \psi \in P_{2N+1-m}$ and any non-negative integer $m \leq 2N+1$, then

$$(\varphi, \psi) = (\varphi, \psi)_N.$$

For any $v \in C(R)$, the Hermite-Gauss interpolant $I_N v \in P_N$ is determined by

$$I_N v(x_j) = v(x_j), \quad 0 \leq j \leq N,$$

Or equivalently,

$$(I_N v - v, \varphi)_N = 0, \quad \forall \varphi \in P_N.$$

3. The fully discrete pseudospectral scheme
$L2-1_{\alpha}$ formula [4] is selected to discretize the Caputo derivative. Set $\tau$ be the step-size in variable $t$, $t_k = k\tau \ (k = 0, 1, \cdots, M; M = \lceil T/\tau \rceil)$, $u^k = u(x, t_k)$. Denote $\alpha = 1 - \frac{\alpha}{2}$

$$a_0^{(\alpha, \sigma)} = \sigma^{1-\alpha}, \quad a_l^{(\alpha, \sigma)} = (l + \sigma)^{1-\alpha} - (l - 1 + \sigma)^{1-\alpha}, l \geq 1,$$

$$b_l^{(\alpha, \sigma)} = \frac{1}{2 - \alpha} [((l + \sigma)^{2-\alpha} - (l - 1 + \sigma)^{2-\alpha}) - \frac{1}{2} ((l + \sigma)^{1-\alpha} - (l - 1 + \sigma)^{1-\alpha}), l \geq 1.$$

For the Caputo derivative we have

$$cD_{0,t}^{ \alpha, \sigma} u(t_{k+\sigma}) = \frac{\tau^{\sigma}}{\Gamma(2-\alpha)} \sum_{j=0}^{k} c_j^{(\sigma, \alpha, \sigma)} (u(t_{k+1-j}) - u(t_{k-j}))) + r_{u,\tau}^{k+\sigma},$$

Where $t_{k+\sigma} = (k + \sigma)\tau, r_{u,\tau}^{k+\sigma}$ is the truncation term $c_0^{(\sigma, \alpha, \sigma)} = a_0^{(\alpha, \sigma)}, \text{for} \ k \geq 1$,
The Numerical experiment.

We consider \( u_N^{k+1} \) by the form of the Lagrangian type interpolants which is on the basis of the Hermite-Gauss nodes \( x_j, j = 0, 1, \ldots, N, \)

\[
u_N^{k+1}(x) = \sum_{j=0}^{N} u_N^{k+1}(x_j) \tilde{h}_j(x),
\]

where \( u_N^{k+1}(x_j) \) are the unknown points of the numerical solution, set \( \tilde{h}_j(x) = h_j(x) e^{-\frac{(x-x_j)^2}{2}} \), \( h_j(x) \) are the Lagrangian polynomials. Substituting \( u_N^{k+1}(x) \) into the discrete scheme (2.2), we can get the linear algebraic system, then it can be easily solved by any traditional numerical method.

**Example.** We consider the numerical problem (1.1)-(1.3) with an exact solution:

\[
u(x, t) = t^{1+\alpha} x \exp(-0.05x^2),
\]

and \( b(x, t) = 2 - \sin(tx), c(x, t) = 2 - \cos(tx). \) The right term is:

\[
f(x, t) = \exp(-0.05x^2)(\Gamma(2 + \alpha)tx + \cos(tx)t^{2+\alpha}(1 - 0.1x^2) + t^{1+\alpha}(2 - \sin(tx)))(0.3x - 0.01x^3) + (2 - \cos(tx)t^{1+\alpha})x).
\]

The \( L^2 \) - errors, \( L^\infty \) - errors and the corresponding convergence rates are shown in Tables 1 and 2. The results are under the condition of \( \alpha = 0.1, 0.5, \alpha = 0.9, \) respectively.

**Table 1.** Numerical results of \( L^2 \) - errors and convergence rates.

| \( \tau \) | \( \alpha = 0.1 \) | \( \alpha = 0.5 \) | \( \alpha = 0.9 \) |
|---|---|---|---|
| Error | Rate | Error | Rate | Error | Rate |
| 1/10 | 1.8830e-04 | * | 3.2724e-03 | * | 9.8748e-03 | * |
| 1/20 | 4.7061e-05 | 2.0004 | 8.1963e-04 | 1.9973 | 2.4626e-03 | 2.0036 |
| 1/40 | 1.1724e-05 | 2.0050 | 2.0546e-04 | 1.9961 | 6.1469e-04 | 2.0023 |
| 1/80 | 2.9150e-06 | 2.0079 | 5.1497e-05 | 1.9963 | 1.5348e-04 | 2.0018 |
| 1/160 | 7.2397e-07 | 2.0095 | 1.2901e-05 | 1.9970 | 3.8331e-05 | 2.0015 |
| 1/320 | 1.7973e-07 | 2.0101 | 3.2306e-06 | 1.9976 | 9.5736e-06 | 2.0014 |
Table 2. Numerical results of $L^\infty$ – errors and convergence rates.

| $\tau$ | $\alpha = 0.1$ | $\alpha = 0.5$ | $\alpha = 0.9$ |
|--------|----------------|----------------|----------------|
|        | Error          | Rate           | Error          | Rate           | Error          |
| 1/10   | 6.5934e-05     | *              | 1.2149e-03     | *              | 3.6610e-03     |
| 1/20   | 1.6457e-05     | 2.0024         | 3.0406e-04     | 1.9985         | 9.1327e-04     | 2.0031         |
| 1/40   | 4.0981e-06     | 2.0056         | 7.6174e-05     | 1.9970         | 2.2802e-04     | 2.0019         |
| 1/80   | 1.0190e-06     | 2.0078         | 1.9083e-05     | 1.9970         | 5.6951e-05     | 2.0014         |
| 1/160  | 2.5316e-07     | 2.0090         | 4.7792e-06     | 1.9975         | 1.4226e-05     | 2.0012         |
| 1/320  | 6.2878e-08     | 2.0094         | 1.1964e-06     | 1.9980         | 3.5539e-06     | 2.0011         |

From Table 1 and Table 2, we clearly see that the accuracy of second-order in time is observed for both $L^2$ – errors and $L^\infty$ – errors at different $\tau$ for given $N$.

Next we give a figure to show the spatial accuracy with the time step size $\tau = 0.001$.

![Figure 1](image1.png)

Figure 1. Errors with $\alpha = 0.1$ for the Example.

![Figure 2](image2.png)

Figure 2. Errors with $\alpha = 0.5$ for the Example.

![Figure 3](image3.png)

Figure 3. Errors with $\alpha = 0.9$ for the Example.

According to Figures 1-3, we find that spectral accuracy in space can be reached at different $N$ for given $\tau$ for both $L^2$ – errors and $L^\infty$ – errors.
5. Conclusions
We establish a fully numerical discrete spectral approximation formula for the equation (1.1)-(1.3) with two variable coefficients on the whole line. We use $L_2 - 1_\sigma$ formula to discretize the Caputo fractional derivative and Hermite functions in space. Numerical results are shown to illustrate the validity and efficiency of the numerical formula (2.2).

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