

## A NOVEL BOX-TYPE SCHEME FOR VARIABLE COEFFICIENT FRACTIONAL SUB-DIFFUSION EQUATION UNDER NEUMANN BOUNDARY CONDITIONS

by

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*In this paper, a novel box-type scheme with convergence order  $O(\tau^{3-\alpha} + h^2)$  is constructed for the fractional sub-diffusion equation with spatially variable coefficient under Neumann boundary conditions. Using  $L_2$  formula and the energy method, stability of the scheme are proved. A numerical example is carried out and the result meets with the theoretical analysis.*

Key words: *fractional sub-diffusion equation,  $L_2$  formula, box-type scheme*

### Introduction

In recent decades, numerous researches were focused on the time fractional sub-diffusion equation (FSDE), which can be derived by applying fractional derivatives to simulate anomalous diffusion.

An efficient approximation for the time fractional derivative is the so-called  $L_1$  method, which came from the piecewise linear interpolate. Sun *et al.* [1] presented a difference scheme for this equation using  $L_1$  approximation, and proved the truncation error to be of  $2 - \alpha$  order in time direction. Zhao *et al.* [2] proposed a box-type scheme for FSDE under Neumann boundary conditions. Applying piecewise quadratic interpolating polynomials, Alikhanov [3] derived a numerical analog (so called  $L_2 - 1_\sigma$  formula) for the Caputo fractional derivative and got order  $O(\tau^{3-\alpha})$ . In [4] the  $L_2 - 1_\sigma$  formula was applied for the time multi-term, and distributed order FSDE. In [5], Alikhanov constructed a  $L_2$  type difference analog for the fractional Caputo derivative with the approximation order  $O(\tau^{3-\alpha})$  in time. Yang [6] suggested the mathematical conjectures for the Fourier integrals with fractional diffusion equation in the sense of Caputo derivative.

Until recently, we find that there are hardly any reports on the difference scheme with accuracy exceeding second order in time direction for FSDE under Neumann boundary condition. In this paper, we aim to construct a box-type difference scheme with the order of  $O(\tau^{3-\alpha})$  in time direction.

### Derivation of the box-type difference scheme

Consider the FSDE under Neumann boundary conditions:

$${}_0^C \mathcal{D}_t^\alpha u(x, t) = \frac{\partial}{\partial x} \left[ \varphi(x) \frac{\partial u}{\partial x} \right] + f(x, t), \quad 0 \leq x \leq L, \quad 0 < t \leq T \quad (1)$$

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$$u(x, 0) = \phi(x), \quad 0 \leq x \leq L \tag{2}$$

$$u_x(0, t) = 0, \quad u_x(L, t) = 0, \quad 0 \leq t \leq T, \tag{3}$$

where

$${}^C_0 \mathcal{D}_t^\alpha f(t) \equiv \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{f'(\xi)}{(t-\xi)^\alpha} d\xi$$

denotes the Caputo fractional derivative and  $\alpha \in (0, 1)$ . We take  $u_x(0, t) = u_x(L, t) = 0$  for simplification. There exists constants  $l_1$  and  $l_2$  such that  $0 < l_1 \leq \phi(x) \leq l_2$ . Giving integers  $M$  and  $N$ , let

$$h = \frac{L}{M}, \quad \tau = \frac{T}{N}, \quad x_i = ih, \quad \Omega_h = \{x_i \mid 0 \leq i \leq M\}, \quad t_n = n\tau, \quad \text{and} \quad \Omega_\tau = \{t_n \mid 0 \leq n \leq N\}$$

We denote

$$U_h = \{u \mid u = (u_0, u_1, \dots, u_M)\} \text{ and } U_{0h} = \{u \mid u = (u_0, u_1, \dots, u_M), u_0 = u_M = 0\}$$

as the grid function spaces. Now we introduce some notation and lemmas for our analysis. Defining:

$$a_l = (l+1)^{1-\alpha} - l^{1-\alpha}, \quad b_l = \frac{1}{2-\alpha} [(l+1)^{2-\alpha} - l^{2-\alpha}] - \frac{1}{2} [(l+1)^{1-\alpha} + l^{1-\alpha}], \quad l \geq 0$$

and

$$c_k^{(2)} = \begin{cases} a_0 + b_0 + b_1, & k = 0 \\ a_1 - b_1 - b_0, & k = 1 \end{cases} \tag{4}$$

$$c_k^{(3)} = \begin{cases} a_0 + b_0, & k = 0 \\ a_1 + b_1 + b_2 - b_0, & k = 1 \\ a_2 - b_2 - b_1, & k = 2 \end{cases} \tag{5}$$

$$c_k^{(n)} = \begin{cases} a_0 + b_0, & k = 0 \\ a_k + b_k - b_{k-1}, & 1 \leq k \leq n-3 \\ a_{n-2} + b_{n-2} + b_{n-1} - b_{n-3}, & k = n-2 \\ a_{n-1} - b_{n-1} - b_{n-2}, & k = n-1 \end{cases} \tag{6}$$

where  $n \geq 4$ . We have the lemmas below for the property of  $a_l, b_l$ , and  $c_k^{(n)}$ .

*Lemma 1.* [5] For any  $\alpha \in (0, 1)$  and  $c_k^{(n)}$  ( $0 \leq k \leq n-1, n \geq 3$ ), it holds that:

$$\frac{\alpha(1-\alpha)}{12(s+1)^{\alpha+1}} \leq b_s \leq \frac{\alpha(1-\alpha)}{12s^{\alpha+1}}$$

$$\frac{11}{16} \cdot \frac{1-\alpha}{n^\alpha} < c_{n-1}^{(n)} < \frac{1-\alpha}{(n-1)^\alpha}$$

$$c_0^{(n)} > c_2^{(n)} > c_3^{(n)} > \dots > c_{n-3}^{(n)} > c_{n-2}^{(n)} > c_{n-1}^{(n)}, \quad c_0^{(n)} + 3c_1^{(n)} - 4c_2^{(n)} > 0$$

For any grid function  $u$ , denote:

$$\Delta_n^\alpha u = \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \left[ c_0^{(n)} u^n - \sum_{j=1}^{n-1} (c_{n-j-1}^{(n)} - c_{n-j}^{(n)}) u^j - c_{n-1}^{(n)} u^0 \right], \quad n \geq 2$$

which is the  $L_2$  formula. For it's error, we have:

$$|{}_0^C D_t^\alpha u(t)|_{t=t_n} - \Delta_{t_n}^\alpha u| = O(\tau^{3-\alpha}), \text{ here } u(t) \in C^3[0, t_n], \quad n \geq 2 \quad [5]$$

Let

$$v(x, t) = \varphi(x) \frac{\partial u}{\partial x}$$

the problem (1)-(3) is equivalent to:

$${}_0^C D_t^\alpha u(x, t) = \frac{\partial}{\partial x} v(x, t) + f(x, t), \quad 0 \leq x \leq L, \quad 0 < t \leq T \quad (7)$$

$$v(x, t) = \varphi(x) \frac{\partial u(x, t)}{\partial x}, \quad 0 \leq x \leq L, \quad 0 \leq t \leq T \quad (8)$$

$$u(x, 0) = \phi(x), \quad 0 \leq x \leq L \quad (9)$$

$$v(0, t) = 0, \quad v(L, t) = 0, \quad 0 < t \leq T \quad (10)$$

We define the grid functions:

$$U_j^n = u(x_j, t_n), \quad V_j^n = v(x_j, t_n), \text{ and denote } f_{j+\frac{1}{2}}^n = f(x_{j+\frac{1}{2}}, t_n)$$

Supposing  $u(x, t) \in C_{x,t}^{(4,3)}([0, L] \times [0, T])$  we consider eqs. (7) and (8) on  $(x_{j+\frac{1}{2}}, t_n)$ , using Taylor expansion see:

$$\Delta_{t_n}^\alpha U_{j+\frac{1}{2}} = \delta_x V_{j+\frac{1}{2}}^n + f_{j+\frac{1}{2}}^n + (R_1)_{j+\frac{1}{2}}^n \quad (11)$$

$$V_{j+\frac{1}{2}}^n = \varphi(x_{j+\frac{1}{2}}) \delta_x U_{j+\frac{1}{2}}^n + (R_2)_{j+\frac{1}{2}}^n \quad (12)$$

where

$$|(R_1)_{j+\frac{1}{2}}^n| \leq C_R(\tau^{3-\alpha} + h^2), \quad |(R_2)_{j+\frac{1}{2}}^n| \leq C_R h^2 \quad (13)$$

Seeing the initial and boundary conditions (9)-(10), and omitting error terms in eqs. (11) and (12), we derive the box-type difference scheme for eqs. (7)-(10):

$$\Delta_{t_n}^\alpha u_{j+\frac{1}{2}} = \delta_x v_{j+\frac{1}{2}}^n + f_{j+\frac{1}{2}}^n, \quad 0 \leq j \leq M-1, \quad 2 \leq n \leq N \quad (14)$$

$$v_{j+\frac{1}{2}}^n = \varphi(x_{j+\frac{1}{2}}) \delta_x u_{j+\frac{1}{2}}^n, \quad 0 \leq j \leq M-1, \quad 0 \leq n \leq N \quad (15)$$

$$v_0^n = 0, \quad v_M^n = 0, \quad 1 \leq n \leq N \quad (16)$$

$$u_j^0 = \phi(x_j), \quad 0 \leq j \leq M \quad (17)$$

### Analysis of the box-type scheme

For  $u, v \in U_h$ , define:

$$\langle u, v \rangle = h \sum_{j=0}^{M-1} u_{j+\frac{1}{2}} v_{j+\frac{1}{2}}, \quad \|u\| = \sqrt{\langle u, u \rangle}, \quad \|\delta_x u\| = \sqrt{\langle \delta_x u, \delta_x u \rangle}$$

$$\langle u, v \rangle_\varphi = h \sum_{j=0}^{M-1} \varphi \left( x_{j+\frac{1}{2}} \right) u_{j+\frac{1}{2}} v_{j+\frac{1}{2}}, \quad \|u\|_\varphi = \sqrt{\langle u, u \rangle_\varphi}, \quad \|u\|_\infty = \max_{0 \leq j \leq M} |u_j|$$

The following *Lemmas* will be helpful for our analysis of the box-type scheme.

*Lemma 2.* [5] For any grid function  $u$  defined on grid  $\Omega_\tau$ , we have:

$$u^n \Delta_{t_n}^\alpha u \geq \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} (\varepsilon_n^{(n)} - \varepsilon_{n-1}^{(n)}) - \frac{\tau^{-\alpha}}{2\Gamma(2-\alpha)} \bar{c}_{n-1}^{(n)} (u^0)^2, \quad 3 \leq n \leq N \tag{18}$$

where

$$\begin{aligned} \bar{c}_0^{(n)} &= \bar{c}_1^{(n)} = c_2^{(n)}, \quad \bar{c}_k^{(n)} = c_k^{(n)}, \quad 2 \leq k \leq n-1 \\ \varepsilon_k^{(n)} &= E_k^{(n)} + \frac{1}{2} \sum_{s=0}^{k-1} \bar{c}_{k-1-s}^{(n)} (u^{s+1})^2, \quad 1 \leq k \leq N \\ E_k^{(n)} &= \left[ \sqrt{\frac{c_0^{(n)} - c_1^{(n)}}{2}} u^k - \left( \frac{1}{2} \sqrt{\frac{c_0^{(n)} - c_1^{(n)}}{2}} + \frac{1}{2} \sqrt{\frac{c_0^{(n)} + 3c_1^{(n)} - 4c_2^{(n)}}{2}} \right) u^{k-1} \right]^2 + \\ &+ \left( \frac{1}{2} \sqrt{\frac{c_0^{(n)} - c_1^{(n)}}{2}} + \frac{1}{2} \sqrt{\frac{c_0^{(n)} + 3c_1^{(n)} - 4c_2^{(n)}}{2}} \right)^2 (u^k)^2, \quad 1 \leq k \leq N \end{aligned}$$

*Lemma 3.* [2] Suppose  $u \in U_h$ , then for any positive constant,  $\epsilon$ , it holds that

$$\|u\|_\infty^2 \leq \left( \epsilon + \frac{h^2}{4L} \right) \|\delta_x u\|^2 + \left( \frac{1}{\epsilon} + \frac{1}{L} \right) \|u\|^2 \tag{19}$$

*Theorem 1.* (Stability) Suppose

$$\{u_j^n \mid 0 \leq j \leq M, 0 \leq n \leq N\}$$

is the solution of the following difference eqs. (14)-(17), then there exists some constant,  $K$ , independent of  $h$ , and  $\tau$ , such that:

$$\tau \sum_{n=5}^N \|u^n\|_\infty^2 \leq K \left[ \sum_{n=0}^4 (\|u^n\|^2 + \|\delta_x u^n\|^2) + \tau \sum_{n=5}^N \|f^n\|^2 \right] \tag{20}$$

*Proof 1.* First we estimate  $\|\delta_x u^n\|$ .

Employing the  $L_2$  approximation operator  $\Delta_{t_n}^\alpha$  and dividing  $\varphi(x_{j+1/2})$  then Multiplying the result by:

$$h v_{j+1/2}^n \text{ to see } \left\langle \Delta_{t_n}^\alpha v, v^n \right\rangle_{1/\varphi} = \left\langle \Delta_{t_n}^\alpha \delta_x u, v^n \right\rangle$$

Multiplying (14) by:

$$h \delta_x v_{j+1/2}^n, \text{ we obtain } \left\langle \Delta_{t_n}^\alpha u, \delta_x v^n \right\rangle = \|\delta_x v^n\|^2 + \left\langle f^n, \delta_x v^n \right\rangle$$

Adding them to give:

$$\|\delta_x v^n\|^2 + \left\langle \Delta_{t_n}^\alpha v, v^n \right\rangle_{1/\varphi} = \left\langle \Delta_{t_n}^\alpha \delta_x u, v^n \right\rangle + \left\langle \Delta_{t_n}^\alpha u, \delta_x v^n \right\rangle - \left\langle f^n, \delta_x v^n \right\rangle \tag{21}$$

Noticing that  $v_0^n = v_M^n = 0$ , we can deduce that

$$\left\langle \Delta_{t_n}^\alpha \delta_x u, v^n \right\rangle + \left\langle \Delta_{t_n}^\alpha u, \delta_x v^n \right\rangle = 0$$

Substituting it into eq. (21), and combining with Cauchy-Schwartz inequality to know:

$$\left\langle \Delta_{t_n}^\alpha v, v^n \right\rangle_{1/\varphi} \leq \frac{1}{4} \|f^n\|^2 \quad (22)$$

From Lemma 2. we know:

$$\left\langle \Delta_{t_n}^\alpha v, v^n \right\rangle_{1/\varphi} \geq \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} (\varepsilon_n^{(n)} - \varepsilon_{n-1}^{(n)}) - \frac{\tau^{-\alpha}}{2\Gamma(2-\alpha)} \bar{c}_{n-1}^{(n)} \|v^0\|_{1/\varphi}^2, \quad 3 \leq n \leq N \quad (23)$$

where

$$\varepsilon_k^{(n)} = E_k^{(n)} + \frac{1}{2} \sum_{s=0}^{k-1} \bar{c}_{k-1-s}^{(n)} \|v^{s+1}\|_{1/\varphi}^2, \quad 1 \leq k \leq N$$

We see that  $c_0^{(n)}, c_1^{(n)}, c_2^{(n)}$  will not change when  $n \geq 5$ , so  $E_k^{(n)} = E_k^{(n+1)}, n \geq 5$ . Noticing that:

$$\bar{c}_k^{(n)} = \bar{c}_k^{(n+1)}, \quad 0 \leq k \leq n-3, \quad n \geq 5$$

so we have:

$$\begin{aligned} \varepsilon_n^{(n)} - \varepsilon_n^{(n+1)} &= E_n^{(n)} - E_n^{(n+1)} + \frac{1}{2} \left[ \sum_{s=0}^{n-1} \bar{c}_{n-1-s}^{(n)} \|v^{s+1}\|_{1/\varphi}^2 - \sum_{s=0}^{n-1} \bar{c}_{n-1-s}^{(n+1)} \|v^{s+1}\|_{1/\varphi}^2 \right] = \\ &= \frac{1}{2} (-2b_{n-1} - b_n) \|v^1\|_{1/\varphi}^2 + \frac{1}{2} b_{n-1} \|v^2\|_{1/\varphi}^2, \quad n \geq 5 \end{aligned} \quad (24)$$

Substituting eq. (23) into eq. (22), and summing up for  $n$  from 5 to  $N$  to give:

$$\frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \left[ \varepsilon_N^{(N)} - \varepsilon_4^{(5)} + \sum_{n=5}^{N-1} (\varepsilon_n^{(n)} - \varepsilon_n^{(n+1)}) \right] - \frac{\tau^{-\alpha}}{2\Gamma(2-\alpha)} \sum_{n=5}^N \bar{c}_{n-1}^{(n)} \|v^0\|_{1/\varphi}^2 \leq \frac{1}{4} \sum_{n=5}^N \|f^n\|^2$$

In view of eq. (24), and notice that  $b_{n-1} > b_n > 0$ , then we have:

$$\begin{aligned} E_N^{(N)} + \frac{1}{2} \sum_{s=0}^{N-1} \bar{c}_{N-1-s}^{(N)} \|v^{s+1}\|_{1/\varphi}^2 &\leq E_4^{(5)} + \frac{1}{2} \sum_{s=0}^3 \bar{c}_{3-s}^{(5)} \|v^{s+1}\|_{1/\varphi}^2 + \frac{3}{2} \|v^1\|_{1/\varphi}^2 \sum_{n=5}^N b_{n-1} + \\ &+ \frac{1}{2} \sum_{n=5}^N \bar{c}_{n-1}^{(n)} \|v^0\|_{1/\varphi}^2 + \frac{\Gamma(2-\alpha)\tau^\alpha}{4} \sum_{n=5}^N \|f^n\|^2 \end{aligned} \quad (25)$$

We have the following estimations.

There exists a constant  $k_1$  independent of  $h$  and  $\tau$ , such that:

$$\begin{aligned} E_4^{(5)} + \frac{1}{2} \sum_{s=0}^3 \bar{c}_{3-s}^{(5)} \|v^{s+1}\|_{1/\varphi}^2 &\leq k_1 \sum_{n=1}^4 \|v^n\|_{1/\varphi}^2 \\ \sum_{s=0}^{N-1} \bar{c}_{N-1-s}^{(N)} \|v^{s+1}\|_{1/\varphi}^2 &\geq \sum_{s=0}^{N-1} \bar{c}_{N-1}^{(N)} \|v^{s+1}\|_{1/\varphi}^2 \geq \frac{11}{16} \frac{1-\alpha}{N^\alpha} \sum_{s=0}^{N-1} \|v^{s+1}\|_{1/\varphi}^2 \\ \sum_{n=5}^N \bar{c}_{n-1}^{(n)} &\leq \sum_{n=5}^N \frac{1-\alpha}{(n-1)^\alpha} = (1-\alpha) \sum_{n=5}^N \int_{n-2}^{n-1} \frac{dx}{(n-1)^\alpha} \\ &\leq (1-\alpha) \sum_{n=5}^N \int_{n-2}^{n-1} \frac{dx}{x^\alpha} = (N-1)^{1-\alpha} - 3^{1-\alpha} < (N-1)^{1-\alpha} \end{aligned}$$

and

$$\begin{aligned} \sum_{n=5}^N b_{n-1} &< \frac{\alpha(1-\alpha)}{12} \sum_{n=5}^N \frac{1}{(n-1)^{\alpha+1}} \leq \frac{\alpha(1-\alpha)}{12} \sum_{n=5}^N \int_{n-2}^{n-1} \frac{dx}{x^{\alpha+1}} = \\ &= \frac{1-\alpha}{12} \left[ \frac{1}{3^\alpha} - \frac{1}{(N-1)^\alpha} \right] < \frac{1-\alpha}{12 \cdot 3^\alpha} \end{aligned}$$

Using these estimations, we have:

$$\begin{aligned} \frac{11}{32} \frac{1-\alpha}{N^\alpha} \sum_{s=0}^{N-1} \|v^{s+1}\|_{1/\varphi}^2 &\leq k_1 \sum_{n=1}^4 \|v^n\|_{1/\varphi}^2 + \frac{1-\alpha}{8 \cdot 3^\alpha} \|v^1\|_{1/\varphi}^2 + \frac{1}{2} (N-1)^{1-\alpha} \|v^0\|_{1/\varphi}^2 + \\ &+ \frac{\Gamma(2-\alpha)\tau^\alpha}{4} \sum_{n=5}^N \|f^n\|^2 \end{aligned} \quad (26)$$

Multiplying it by  $N^\alpha \tau$ , and seeing eq. (15), we know there exists a constant  $K_1$  such that:

$$\tau \sum_{n=5}^N \|\delta_x u^n\|^2 \leq K_1 \left( \sum_{n=0}^4 \|\delta_x u^n\|^2 + \tau \sum_{n=5}^N \|f^n\| \right) \quad (27)$$

Applying the similar analysis to estimate  $\|u^n\|$ , and seeing *Lemma 3*, we get eq. (20) and finish the proof.

Using the similar analysis, we can get convergence for the scheme (14)-(17).

*Theorem 2. (Convergence) Suppose*

$$u(x, t) \in C_{x,t}^{(4,3)}([0, L] \times [0, T])$$

is the exact solution of problem (1)-(3). Let

$$U_j^n = u(x_j, t_n), \quad e_j^n = U_j^n - u_j^n$$

then we have

$$\tau \sum_{n=5}^N \|e^n\|_\infty \leq O(\tau^{3-\alpha} + h^2) \quad (28)$$

## Numerical experience

*Example 1.* We take

$$L = T, \quad \varphi(x) = e^{-x}, \quad \text{and} \quad f(x, t) = e^{2x} \frac{\Gamma(4+\alpha)}{6} t^3 - 2e^x t^{3+\alpha}$$

for the problem (1)-(3), then the exact solution is

$$u(x, t) = e^{2x} t^{3+\alpha}.$$

We solve the problem with scheme (14)-(17). The convergence order in temporal is tested by taking fixed spatial step  $h = 1/20000$ . The computational errors and convergence

orders in the maximum norm are listed in tab. 1. The results are consistent with our theoretical analysis.

**Table 1. The error and convergence order in temporal direction with  $h = 1/20000$**

$\tau$	$\alpha = 0.2$		$\alpha = 0.5$		$\alpha = 0.8$	
	$E_x(h, \tau)$	Order ( $\tau$ )	$E_x(h, \tau)$	Order ( $\tau$ )	$E_x(h, \tau)$	Order ( $\tau$ )
1/10	$2.0512 \cdot 10^{-3}$	*	$1.4179 \cdot 10^{-2}$	*	$5.7486 \cdot 10^{-2}$	*
1/20	$3.3342 \cdot 10^{-4}$	2.6210	$2.8559 \cdot 10^{-3}$	2.3117	$1.4386 \cdot 10^{-2}$	1.9986
1/40	$5.1631 \cdot 10^{-5}$	2.6910	$5.3520 \cdot 10^{-4}$	2.4158	$3.3058 \cdot 10^{-3}$	2.1216
1/80	$7.7652 \cdot 10^{-6}$	2.7331	$9.7472 \cdot 10^{-5}$	2.4570	$7.3627 \cdot 10^{-4}$	2.1667
1/160	$1.1203 \cdot 10^{-6}$	2.7931	$1.7564 \cdot 10^{-5}$	2.4723	$1.6197 \cdot 10^{-4}$	2.1845
1/320	$1.4880 \cdot 10^{-7}$	2.9125	$3.1526 \cdot 10^{-6}$	2.4780	$3.5456 \cdot 10^{-5}$	2.1916

### Conclusion

In this paper, we construct a box-type difference scheme with convergence order  $O(\tau^{3-\alpha} + h^2)$  for FSDE which has Neumann boundary conditions. Using  $L_2$  formula, we get the stability and convergency of the scheme. A numerical example is implemented to testify the scheme.

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