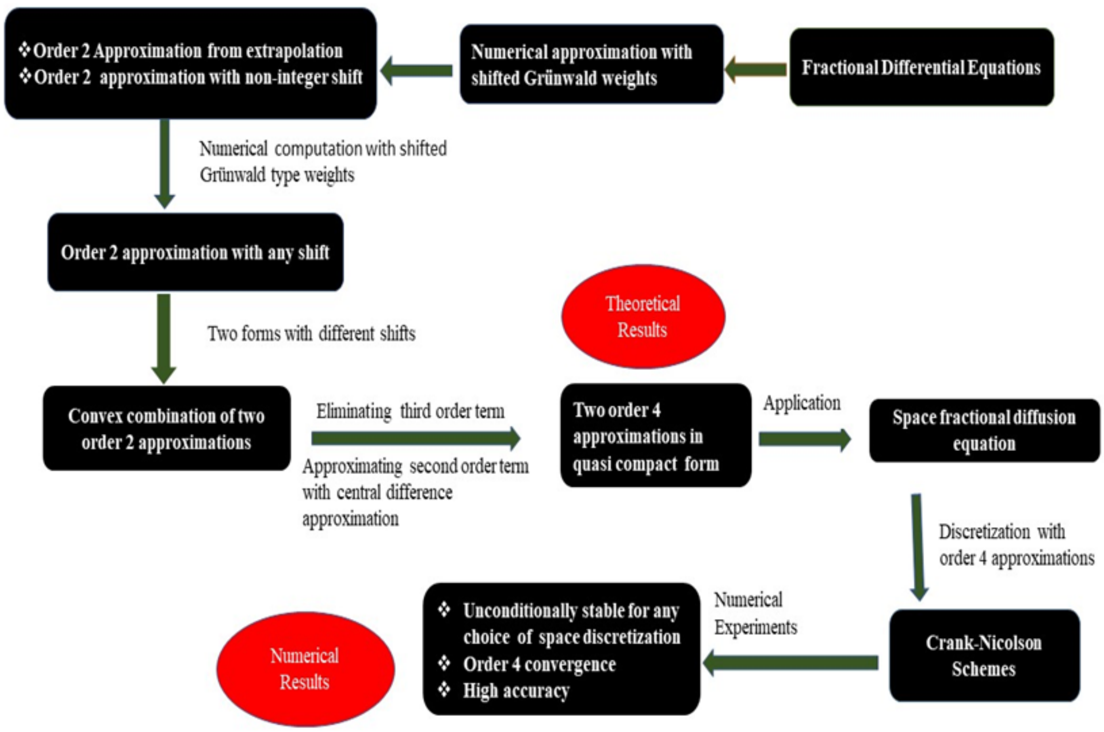
Ceylon Journal of Science 51(Special Issue) 2022: 589-595

RESEARCH ARTICLE

Quasi-compact fourth-order approximations for fractional derivatives and applications

W. A. Gunarathna*, H. M. Nasir and W. B. Daundasekara



Highlights

- Two new fourth-order approximations for fractional derivatives with the shift.
- The second-order approximation with shift plays a central role.
- Application in Crank-Nicolson schemes to the fractional diffusion equation.
- The Crank-Nicolson schemes are unconditionally stable.

Ceylon Journal of Science 51 (Special Issue) 2022: 589-595
DOI: http://doi.org/10.4038/cjs.v51i5.8085

RESEARCH ARTICLE

Quasi-compact fourth-order approximations for fractional derivatives and applications

W. A. Gunarathna[1, 2*], H. M. Nasir[3] and W. B. Daundasekara[4]

[1]*Department of Physical Sciences, Faculty of Applied Science, Rajarata University of Sri Lanka*
[2]*Postgraduate Institute of Science, University of Peradeniya, Peradeniya, Sri Lanka*
[3]*FracDiff Research Group, Department of Mathematics, College of Science, Sultan Qaboos University, Sultanate of Oman*
[4]*Department of Mathematics, Faculty of Science, University of Peradeniya, Peradeniya, Sri Lanka*

Received: 30/06/2021; Accepted:04/02/2022

Abstract: Two fourth-order approximations for fractional derivatives are presented. These approximations are constructed from an approximation of order 2 through convex combinations of two different shifts eliminating the third-order term and then approximating the remaining second-order term with a central difference approximation. The constructed approximations are applied in Crank-Nicolson schemes to the one-dimensional space fractional diffusion equation. Numerical tests confirm that the schemes are unconditionally stable for any choice of space discretization and converge with order 4.

***Keywords*:** Fractional derivatives; generating functions; grünwald approximation; Crank-Nicolson scheme; fractional diffusion equations.

INTRODUCTION

Fractional derivatives have recently been used in numerous real-world applications in many branches of science and engineering including fractal phenomena, anomalous diffusion, viscoelasticity, and biological population models (Koeller, 1984; Rossikhin and Shitikova, 1997; Metzler and Klafter, 2004; Sun *et al*., 2018). There are different types of fractional derivatives that have been presented in the literature, of which the Grünwald-Letnikov derivative is often employed to approximate the Riemann-Liouville (R-L) fractional derivative (Podlubny, 1998; Diethelm, 2010). These fractional derivatives are non-local operators in the sense that a fractional derivative at a point involves function values spread throughout the domain; thus, numerical computation of the derivatives becomes an involved computational task.

For a sufficiently smooth function f defined on the real line domain, the left (-) and right (+) Riemann-Liouville (R-L) fractional derivatives of order $\alpha > 0$ are defined by

$$D_{x-}^{\alpha} f(x) = \frac{1}{\Gamma(n-\alpha)} \frac{d^n}{dx^n} \int_{-\infty}^{x} \frac{f(\xi)}{(x-\xi))^{\alpha+1-n}} d\xi$$

and

$$D_{x+}^{\alpha} f(x) = \frac{(-1)^n}{\Gamma(n-\alpha)} \frac{d^n}{dx^n} \int_{x}^{\infty} \frac{f(\xi)}{(\xi-x))^{\alpha+1-n}} d\xi, \quad (1)$$

respectively, where $\Gamma(\cdot)$ is the Gamma function and $n = [\alpha] + 1$, where $[\alpha]$ denotes the integer part of α.

Grünwald approximation (GA) of (1) is a basic formulation that is commonly used to approximate the R-L fractional derivatives (Podlubny, 1998). The shifted Grünwald approximation for the left and right R-L fractional derivatives is given by

$$\delta_{h-,r}^{\alpha} f(x) = \frac{1}{h^{\alpha}} \sum_{k=0}^{\infty} g_k^{(\alpha)} f(x-(k-r)h)$$

and

$$\delta_{h+,r}^{\alpha} f(x) = \frac{1}{h^{\alpha}} \sum_{k=0}^{\infty} g_k^{(\alpha)} f(x+(k-r)h), \quad (2)$$

respectively.

The weight coefficients

$g_k^{(\alpha)} = (-1)^k \ \Gamma(n+1)/(k!\,\Gamma(\alpha+1-k))$ are the coefficients of the power series expansion of the generating function $W_1(z) = (1-z)^{\alpha}$ and r is the shift parameter. The GA is of the first-order accuracy, and when applied to the space-fractional diffusion equation (SFDE) without shift ($r = 0$), it displays unstable solutions for the implicit Euler and Crank-Nicolson (C-N) methods which are well-known for their unconditional stability for classical diffusion problems. Its shifted form with shift $r = 1$ restores the stability in these methods with the same first-order accuracy (Meerschaert and Tadjeran, 2004).

Lubich (1986) derives a class of some higher-order Grünwald type approximations in terms of generating functions of the form

$$W_p(z) = \left(\sum_{k=1}^{p} \frac{1}{k} (1-z)^k \right)^{\alpha} ; p = 1,2,\dots,6. \quad (3)$$

**Corresponding Author's Email: anura@as.rjt.ac.lk*
https://orcid.org/0000-0002-2163-3929

In these cases, the coefficients $g_k^{(\alpha)}$ in (2) are replaced by the coefficients of the Taylor series expansion of the Lubich generating functions in (3) without shift ($r = 0$) to obtain higher-order approximations. Numerical experiments show that these approximations also suffer similar stability issues as in the case of GA. The shifted form (2) with the Lubich coefficients restores the stability; however, it brings the order of accuracy down to one and hence, becomes less beneficial. Therefore, in the literature, higher-order approximations for fractional diffusion problems have mostly utilized the first-order GA in (2).

Since the C-N approximation is of the second-order accuracy in time step τ, and (2) gives only first-order accuracy in space step h, Tadjeran *et al*. (2006) developed a second-order accurate approximation for the space discretization using extrapolation improvement. Nasir *et al*. (2013) derived a second-order approximation with superconvergence using (2) with a non-integer shift $r = \alpha/2$. Some other higher-order approximations were obtained by using convex combinations of two or three mutually different shifted forms of (2). This technique is called the weighted and shifted Grünwald difference (WSGD) (Zhou, *et al*., 2013). In Tian *et al*. (2015), by using the WSGD technique, some-second order approximations were established and applied to solve space fractional diffusion equations with unconditional stability for $1 < \alpha < 2$. Hao *et al*. (2015) obtained a fourth-order approximation through a quasi-compact approximation (QCA). All the foregoing approximations are developed from the first-order GA only.

Nasir and Nafa (2018a) proposed a new set of Grünwald type higher-order approximations that retain the higher orders with an arbitrary shift r. These generating functions are in the form of power of polynomial viewed by

$$W_{p,r}(z) = \left(b_0 + b_1 z + b_2 z^2 + \cdots + b_p z^p\right)^{\alpha}, \tag{4}$$

where p is the accuracy order and $b_j = b_j(\alpha, r), j = 1, 2, \ldots, p$.

It is proved and numerically verified in Nasir and Nafa (2018a) that the second-order approximation is reliable with $1 < \alpha < 2$ for stability and consistency. The corresponding generating function for the second-order approximation with shift r is given by

$$W_{2,r}(z) = \left(\frac{3}{2} - \frac{r}{\alpha} + \left(-2 + \frac{r}{\alpha}\right) z + \left(\frac{1}{2} - \frac{r}{\alpha}\right) z^2\right)^{\alpha}. \tag{5}$$

Nasir and Nafa (2018b) used the second-order approximation along with the quasi-compact technique to obtain a third-order approximation and applied it to seek a numerical solution of the one-dimensional space fractional diffusion equation with unconditional stability for the C-N scheme. An explicit form for the generating functions of the shifted Grünwald difference for any finite order p and arbitrary real shift r was presented by the authors (Gunarathna *et al*., 2019). For a review of difference approximations for fractional derivatives, we direct the reader to (Cai and Li, 2020). In this study, we mainly develop two new fourth-order Grünwald type approximations for the R-L derivatives using the second-order approximation $W_{2,r}(z)$ in (5). We then apply these approximations in the C-N type scheme for the SFDE.

MATERIALS AND METHODS

Preliminary preparation

In this section, we summarize, some properties of the Fourier transform, the theories established in Nasir and Nafa (2018a) and Gunarathna *et al*. (2019) for constructing approximate generating functions with shifts.

Fourier transform

Definition 1. The Fourier (FT) of an integrable function $f \in L_1(\Omega)$, where $\Omega \subseteq \mathbb{R}$ is given by

$$\mathcal{F}[f(x)](\eta) =: \hat{f}(\eta) = \int_{\Omega} f(x) e^{-i\eta x}\, dx.$$

The corresponding inverse Fourier transform(IFT) is given by

$$\mathcal{F}^{-1}[\hat{f}(\eta)](x) = \int_{\Omega} \hat{f}(\eta) e^{i\eta x}\, d\eta = f(x).$$

We list below some properties of FT that will be used in this paper.

Preposition 1. Let $f, g, D_{x-}^{\alpha} f$, and $D_{x+}^{\alpha} f$ be in $L_1(\Omega)$ with $\mathcal{F}[f(x)](\eta) = \hat{f}(\eta)$ and $\mathcal{F}[g(x)](\eta) = \hat{g}(\eta)$.

a. The FT satisfies the linearity:

$$\mathcal{F}[c_1 f(x) + c_2 g(x)](\eta) = c_1 \hat{f}(\eta) + c_2 \hat{g}(\eta), c_1, c_2 \in \mathbb{R}.$$

b. The FT satisfies the shift property,

$$\mathcal{F}[f(x+c)](\eta) = e^{ic\eta} \hat{f}(\eta), \qquad c \in \mathbb{R}.$$

c. The FTs of the left and right fractional derivatives are given by

$$\mathcal{F}[D_{x-}^{\alpha} f(x)](\eta) = (i\eta)^{\alpha} \hat{f}(\eta) \text{ and } \mathcal{F}[D_{x+}^{\alpha} f(x)](\eta) = (-i\eta)^{\alpha} \hat{f}(\eta),$$

respectively (Podlubny, 1998).

General Grünwald type approximations

Definition 2. For a sufficiently smooth function f and generic weights $w_{k,r}^{(\alpha)}$, the left and right Grünwald-type operators with shift r are defined as

$$\Delta_{h-,r,p}^{\alpha} f(x) = \frac{1}{h^{\alpha}} \sum_{k=0}^{\infty} w_{k,r}^{(\alpha)} f(x - (k-r)h)$$

and

$$\Delta_{h+,r,p}^{\alpha} f(x) = \frac{1}{h^{\alpha}} \sum_{k=0}^{\infty} w_{k,r}^{(\alpha)} f(x + (k-r)h), \tag{6}$$

respectively, where h is the subinterval size of a uniform partition of the domain of $f(x)$.

Definition 3. Let $W(z)=\sum_{k=0}^{\infty} w_k^{(\alpha)} z^k$ be the generating function of a real sequence $\{w_k^{(\alpha)}\}$.

a. $W(z)$ is said to approximate the left or right fractional derivative $D_{x\mp}^{\alpha} f(x)$ at x with shift r in the Grünwald sense if

$$D_{x\mp}^{\alpha} f(x)=\lim_{h\to 0} \Delta_{x\mp h,r}^{\alpha} f(x).$$

b. $W(z)$ is said to approximate $D_{x\mp}^{\alpha} f(x)$ with order $p\geq 1$ and shift r at x if

$$\Delta_{\mp h,r,p}^{\alpha} f(x)=D_{x\mp}^{\alpha} f(x)+O(h^p). \quad (7)$$

Theorem 1. ((Nasir & Nafa, 2018 a)) Let $n=[\alpha]+1$, m a non-negative integer, $f\in C^{m+n+1}(\mathbb{R})$ and $D_x^k f=\frac{d^k}{dx^k} f\in L_1(\mathbb{R})$ for integer k, $0\leq k\leq m+n+1$. Then the generating function W approximates the left or right fractional differential operator $D_{x\mp}^{\alpha}$ with order p and shift r, $1\leq p\leq m$, if and only if

$$G_p(z)=\frac{1}{z^{\alpha}} W(e^{-z}) e^{rz}$$

is analytic in a disk $|z|\leq R$ for some $R>0$ and

$$G_p(z)=1+O(z^p). \quad (8)$$

Moreover, if $G_p(z)=1+\sum_{l=p}^{\infty} a_l(r) z^l$, we then have

$$\Delta_{h\mp,r,p}^{\alpha} f(x)=D_{x\mp}^{\alpha} f(x)+h^p a_p(r) D_{x\mp}^{\alpha+p} f(x)+\cdots+O(h^m). \quad (9)$$

The following corollary is a direct consequence of this theorem.

Corollary 1. If the generating function $W(z)$ approximates the fractional derivatives, then $W(1)=0$. This means that $\sum_{k=0}^{\infty} w_k^{(\alpha)}=0$.

Proof.

For $z\neq 0$, Equation (8) gives

$$G_p(z)=\frac{1}{z^{\alpha}} W(e^{-z}) e^{rz}=1+O(z^p).$$

Hence, we have $W(e^{-z}) e^{rz}=z^{\alpha}\left(1+O(z^p)\right)$.

Letting $z\to 0$, we have $W(1)=0$. ■

Theorem 2. ((Gunarathna, et al., 2019)) The generating function $W(z)=\left(\sum_{j=0}^{p} b_j z^j\right)^{\alpha}$ approximates the fractional differential operator $D_{x\mp}^{\alpha}$ with shift r and order p if and only if the coefficients b_j are given by

$$b_j=-\left(\sum_{\substack{m=0\\ m\neq j}}^{p} \prod_{\substack{l=0\\ l\neq m,j}}^{p} (\lambda-l)\right)\left(\prod_{\substack{m=0\\ m\neq j}}^{p} \frac{1}{j-m}\right), \quad j=0,1,2,\dots,p, \quad (10)$$

where $\lambda=r/\alpha$. The leading error constant is given by

$$E_p=\frac{\alpha}{(p+1)!}\sum_{j=0}^{p} (\lambda-j)^{p+1} b_j. \quad (11)$$

For $p=2$, that is, for a second-order approximation $W_2(z)=\left(\sum_{j=0}^{2} b_j z^j\right)^{\alpha}$, (10) yields the coefficients b_j such that

$$b_0=\frac{3}{2}-\lambda,\ b_1=-2+2\lambda,\ b_2=\frac{1}{2}-\lambda. \quad (12)$$

Then Equation (9) with $p=2$ and a function $f\in C^{m+n+1}(\mathbb{R})$ gives

$$\Delta_{\mp h,r,2}^{\alpha} f(x)=D_{x\mp}^{\alpha} f(x)+h^2 a_2(r) D_{x\mp}^{\alpha+2} f(x)+\cdots+O(h^m). \quad (13)$$

Further, Corollary 1 confirms that $(1-z)$ is a factor of $P_2(z)=\sum_{j=0}^{2} b_j z^j$; thereby we can express $W_2(z)$ as

$$W_2(z)=(1-z)^{\alpha}(b_0-b_2 z)^{\alpha}. \quad (14)$$

To have real weight coefficients $w_{j,r}^{(\alpha)}$ for $W_2(z)=\sum_{j=0}^{\infty} w_{j,r}^{(\alpha)} z^j$, we must have $b_0=3/2-\lambda>0$, so $\lambda<3/2$. The power series converges to zero at $z=1$, due to Corollary 1. For the power series to be convergent to $W_2(z)$, we must have

$$0<\left|\frac{b_2}{b_0} z\right|<1 \text{ and } 0<|z|\leq 1. \quad (15)$$

Then, from (15), we have the resulting convergence when $\lambda<1$ or $\alpha>r$.

The coefficient $w_j^{(\alpha)}$ of the generating function $\sum_{j=0}^{\infty} w_{j,r}^{(\alpha)} z^j$ can be computed using the J. C. P. Miller recurrence such that

$$w_{0,r}^{(\alpha)}=b_0{}^{\alpha},$$

$$w_{1,r}^{(\alpha)}=\alpha b_0{}^{\alpha-1} b_1,$$

$$w_{j,r}^{(\alpha)}=\frac{1}{j b_0}\left[(\alpha+1-j) w_{j-1,r}^{(\alpha)} b_1+(2\alpha+2-j) w_{j-2,r}^{(\alpha)} b_2\right],$$

for $j=2,3,\dots$, where $\alpha>r$. (16)

Fourth-order approximations

In this section, we present our main results by constructing two fourth-order approximations for the R-L fractional derivatives in (1). Both the approximations are of QCA type. Our construction is analogous to the work of Hao *et al.* (2015). We first derive the approximations for the left fractional derivatives in (1).

Let $f\in C^{n+5}(\mathbb{R})$, and consider two approximations of (13) with two different shifts r_1, r_2.

We then have:

$$\Delta^{\alpha}_{h-,r_1,2} f(x) = D^{\alpha}_{x-} f(x) + h^2 a_2(r_1) D^{\alpha+2}_{x-} f(x) + h^3 a_3(r_1) D^{\alpha+3}_{x-} f(x) + O(h^4) \quad (17)$$

$$\Delta^{\alpha}_{h-,r_2,2} f(x) = D^{\alpha}_{x-} f(x) + h^2 a_2(r_2) D^{\alpha+p}_{x-} f(x) + h^3 a_3(r_2) D^{\alpha+3}_{x-} f(x) + O(h^4), \quad (18)$$

where

$$a_2(r) = \frac{r^2}{2\alpha} + r - \frac{\alpha}{3}, \qquad a_3(r) = \frac{r^3}{3\alpha^2} + \frac{r^2}{\alpha} - \frac{11r}{12} + \frac{\alpha}{4}.$$

A linear combination of (18) and (19) gives an approximation operator A_{r_1,r_2-} as

$$A_{r_1,r_2-} f(x) = (\mu_1 + \mu_2) D^{\alpha}_{x-} f(x) + \big(\mu_1 a_2(r_1) + \mu_2 a_2(r_2)\big) h^2 D^{\alpha+2}_{x-} f(x) + \big(\mu_1 a_3(r_1) + \mu_2 a_3(r_2)\big) h^3 D^{\alpha+3}_{x-} f(x) + O(h^4), \quad (19)$$

where

$$A_{r_1,r_2-} f(x) = \big(\mu_1 \Delta^{\alpha}_{h-,r_1,2} + \mu_2 \Delta^{\alpha}_{h-,r_2,2}\big) f(x).$$

Correspondingly, its generating function is given by $V(z) = \mu_1 W_{2,r_1}(z) + \mu_2 W_{2,r_2}(z)$.

If $V(z)$ is to approximate the fractional derivative with order 2, we have by Theorem 1,

$$G(z) = \mu_1 \frac{1}{z^{\alpha}} W_{2,r_1}(e^{-z}) e^{r_1 z} + \frac{1}{z^{\alpha}} \mu_2 W_{2,r_2}(e^{-z}) e^{r_2 z}$$

$$= (\mu_1 + \mu_2) + \sum_{l=2}^{\infty} \big(\mu_1 a_l(r_1) + \mu_2 a_l(r_2)\big) z^l = 1 + O(z^2).$$

We thus get the linear system:

$$\begin{aligned} \mu_1 + \mu_2 &= 1, \\ \mu_1 a_3(r_1) + \mu_2 a_3(r_2) &= 0, \end{aligned}$$

with leading error coefficient

$$l_2(r_1,r_2) = \mu_1 a_2(r_1) + \mu_2 a_2(r_2).$$

Solving the foregoing system with the choice of shift combination (r_1, r_2), we have:

$$l_2(r_1,r_2)$$

$$\frac{4\alpha^4 - 15\alpha^3 r_1 - 15\alpha^3 r_2 + 8\alpha^2 r_1^2 + 47\alpha^2 r_1 r_2 + 8\alpha^2 r_2^2 - 24\alpha r_1^2 r_2 - 24\alpha r_1 r_2^2 + 12 r_1^2 r_2^3}{6\alpha(11\alpha^2 - 12\alpha r_1 - 12\alpha r_2 + 4r_1^2 + 4r_1 r_2 + 4r_2^2)}$$

$$= -$$

$$\mu_1 = \frac{(-3\alpha + 2r_2)(-\alpha + r_2)(-\alpha + 2r_2)}{(r_1 - r_2)(11\alpha^2 - 12\alpha r_1 - 12\alpha r_2 + 4r_1^2 + 4r_1 r_2 + 4r_2^2)},$$

$$\mu_2 = 1 - \mu_1.$$

From the above derivation, we have for the shift combinations $(r_1, r_2) = (1, 0)$ and $(r_1, r_2) = (-1, 1)$:

$$\mu_1(1,0) = \frac{3\alpha^3}{11\alpha^2 - 12\alpha + 4},$$

$$\mu_2(1,0) = \frac{-3\alpha^3 + 11\alpha^2 - 12\alpha + 4}{11\alpha^2 - 12\alpha + 4}, \quad (20)$$

$$l_2(1,0) = \frac{-4\alpha^3 + 15\alpha^2 - 8\alpha}{6(11\alpha^2 - 12\alpha + 4)}; \quad (21)$$

and

$$\mu_1(1,-1) = \frac{3\alpha^3 + 11\alpha^2 + 12\alpha + 4}{22\alpha^2 + 8},$$

$$\mu_2(1,-1) = \frac{-3\alpha^3 + 11\alpha^2 - 12\alpha + 4}{22\alpha^2 + 8}, \quad (22)$$

$$l_2(1,-1) = \frac{-4\alpha^4 + 31\alpha^2 - 12}{6\alpha(11\alpha^2 + 4)}, \quad (23)$$

respectively.

We then have from (19) with the preceding shift combinations that

$$\begin{aligned} A_{r_1,r_2-} f(x) &= D^{\alpha}_{x-} f(x) + l_2(r_1,r_2) h^2 D^{\alpha+2}_{x-} f(x) + O(h^4) \\ &= (I + l_2(r_1,r_2) h^2 D^2_x) D^{\alpha}_{x-} f(x) + O(h^4) \\ &= L_x D^{\alpha}_{x-} f(x) + O(h^4), \end{aligned} \quad (24)$$

where $L_x = I + l_2(r_1,r_2) h^2 D^2_x$ and I denotes the identity operator.

With the uniform discretization of the domain with subinterval size h, the second derivative is approximated by the central difference approximation such that

$$D^2_x f(x) = \delta^2_h f(x) + O(h^2),$$

where $\delta^2_h f(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$.

We then get

$$\begin{aligned} L_x f(x) &= (I + l_2(r_1,r_2) h^2 (\delta^2_h + O(h^2))) f(x) + O(h^4) \\ &= L_h f(x) + O(h^4), \end{aligned} \quad (25)$$

where $L_h = I + l_2(r_1,r_2) h^2 \delta^2_h$.

Then Equations (24) and (25) confirm that the operator $L_x D^{\alpha}_{x-}$ is approximated by A_{r_1,r_2} with order 4 accuracy, and similarly, we can also establish the analogous construction for the right fractional derivative as viewed in (26):

$$\begin{aligned} & A_{r_1,r_2-} f(x) = L_x D^{\alpha}_{x-} f(x) + O(h^4), \\ & (r_1, r_2) = (1,0), (1,-1) \\ & A_{r_1,r_2+} f(x) = L_x D^{\alpha}_{x+} f(x) + O(h^4), \\ & (r_1, r_2) = (1,0), (1,-1). \end{aligned} \quad (26)$$

The leading error term $R_4(r_1,r_2)$ of the approximation (26) is given by, for shifts (1,0),

$$R_4(1,0) = -\frac{140\alpha^4 - 698\alpha^3 + 1246\alpha^2 - 967\alpha + 270}{360(11\alpha^2 - 12\alpha + 4)} h^4 D^{\alpha+4}_{x-} f(\xi)$$

and for (1,-1),

$$R_4(1,-1) = \frac{-140\alpha^7 + 218\alpha^6 + 740\alpha^5 - 1178\alpha^4 - 705\alpha^3 + 1290\alpha^2 + 180\alpha - 360}{360\alpha^3(11\alpha^2+4)} h^4 D_{x-}^{\alpha+4} f(\xi),$$

where $\xi \in (-\infty, x)$.

Applications

For an application of our proposed schemes, we consider the numerical approximation of the space fractional diffusion equation in the domain $[a,b] \times [0,T]$:

$$\frac{\partial u(x,t)}{\partial t} = K_1 D_{x-}^{\alpha} u(x,t) + K_2 D_{x+}^{\alpha} u(x,t) + f(x,t), \quad (27)$$

with the initial and boundary conditions:

$$u(x,0) = S_0(x), \quad x \in [a,b], \quad (28)$$

$$u(a,t) = \phi_1(t), \quad u(b,t) = \phi_2(t), \quad t \in [0,T], \quad (29)$$

where $u(x,t)$ is the unknown function to be determined; K_1 and K_2 are non-negative diffusion constants with $K_1 + K_2 \neq 0$; and $f(x,t)$ is a known source function.

The function $u(x,t)$ is zero-extended outside the space domain $[a,b]$ so that the left and right fractional derivatives are applicable.

The space domain is partitioned into a uniform mesh of size N with grid size $h = (b-a)/N$, and so is the time domain into a uniform partition of size M with grid size $\tau = T/M$.

These form the uniform partition $[a,b] \times [0,T]$ with grid points (x_i, t^m), where $x_i = a + ih$ and $t^m = m\tau$, for all pairs (i,m), $0 \le i \le N, 0 \le m \le T$.

We employ the following notations:

$$u_i^m = u(x_i, t^m),\ t^{m+1/2} = \tfrac{1}{2}(t^{m+1} + t^m) \text{ and}$$

$$f_i^{m+1/2} = f\left(x_i, t^{m+1/2}\right).$$

Pre-multiplying (27) by L_h gives

$$L_h \frac{\partial u(x,t)}{\partial t} = K_1 L_h D_{x-}^{\alpha} u(x,t) + K_2 L_h D_{x+}^{\alpha} u(x,t) + L_h f(x,t).$$

To construct the C-N scheme, we write the FDE at $(x, t+\tau/2)$, and approximate the time derivative by the second-order central difference scheme

$$\frac{\partial u(x,t+\tau/2)}{\partial t} = \frac{1}{\tau}(u(x,t+\tau) - u(x,\tau)) + O(\tau^2)$$

and the left and right fractional derivatives are given by (26), respectively. We then have shift combinations $(r_1,r_2) = (1,0),(1,-1)$

$$\frac{1}{\tau}(u(x,t+\tau) - u(x,\tau)) = \frac{1}{\tau} B_h(u(x,t+\tau) - u(x,\tau)) + O(h^4 + \tau^2), \quad (30)$$

where $B_h = B_h(r_1,r_2) = K_1 \Delta_{h-,r_1,r_2,2}^{\alpha} + K_2 \Delta_{h+,r_1,r_2,2}^{\alpha}$.

The matrix form of the C-N scheme is given by

$$(L_\alpha - B_\alpha) U^{m+1} = (L_\alpha + B_\alpha) U^m + \tau L_\alpha F^{m+1/2} + O(\tau^3 + \tau h^4) \quad (31)$$

for all $m = 1, 2, \dots, M-1$, where

$$U^m = [u_0^m, u_1^m, \cdots, u_N^m]^T,$$

$$F^{m+1/2} = [f_0^{m+1/2}, f_1^{m+1/2}, \cdots, f_N^{m+1/2}]^T,$$

and L_α is a triangular matrix of size $N+1$ and B_α is a matrix of the same size that is given by

$$L_\alpha = \frac{\tau}{2} \mathrm{Tri}[A_2(r_1,r_2), 1 - 2A_2(r_1,r_2), A_2(r_1,r_2)],$$

$$B_\alpha = \frac{\tau}{2}\left[\mu_1(r_1,r_2)\left(K_1 A_{r_1,2} + K_2 A_{r_1,2}{}^T\right) + \mu_2(r_1,r_2)\left(K_1 A_{r_2,2} + K_2 A_{r_2,2}{}^T\right)\right],$$

where $A_{r,2}, r = -1,0,1$ are Toeplitz matrices, formed by the respective weight coefficients computed using (16), are given below:

$$A_{1,2} = \frac{1}{h^\alpha}\begin{pmatrix} w_{1,1}^{(\alpha)} & w_{0,1}^{(\alpha)} & 0 & 0 & \cdots & 0 & 0 \\ w_{2,1}^{(\alpha)} & w_{1,1}^{(\alpha)} & w_{0,1}^{(\alpha)} & 0 & \cdots & 0 & 0 \\ w_{3,1}^{(\alpha)} & w_{2,1}^{(\alpha)} & w_{1,1}^{(\alpha)} & w_{0,1}^{(\alpha)} & \ddots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & 0 & \vdots \\ w_{N-1,1}^{(\alpha)} & w_{N-2,1}^{(\alpha)} & w_{N-3,1}^{(\alpha)} & \cdots & \ddots & w_{0,1}^{(\alpha)} & 0 \\ w_{N,1}^{(\alpha)} & w_{N-1,1}^{(\alpha)} & w_{N-2,1}^{(\alpha)} & \cdots & w_{2,1}^{(\alpha)} & w_{1,1}^{(\alpha)} & w_{0,1}^{(\alpha)} \\ w_{N+1,1}^{(\alpha)} & w_{N,1}^{(\alpha)} & w_{N-1,1}^{(\alpha)} & \cdots & w_{3,1}^{(\alpha)} & w_{2,1}^{(\alpha)} & w_{1,1}^{(\alpha)} \end{pmatrix},$$

$$A_{0,2} = \frac{1}{h^\alpha}\begin{pmatrix} w_{0,0}^{(\alpha)} & 0 & 0 & 0 & \cdots & 0 & 0 \\ w_{1,0}^{(\alpha)} & w_{0,0}^{(\alpha)} & 0 & 0 & \cdots & 0 & 0 \\ w_{2,0}^{(\alpha)} & w_{2,0}^{(\alpha)} & w_{0,0}^{(\alpha)} & 0 & \ddots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & 0 & \vdots \\ w_{N-2,0}^{(\alpha)} & w_{N-3,0}^{(\alpha)} & w_{N-4,0}^{(\alpha)} & \cdots & \ddots & 0 & 0 \\ w_{N-1,0}^{(\alpha)} & w_{N-2,0}^{(\alpha)} & w_{N-2,0}^{(\alpha)} & \cdots & w_{1,0}^{(\alpha)} & w_{0,0}^{(\alpha)} & 0 \\ w_{N,0}^{(\alpha)} & w_{N-1,0}^{(\alpha)} & w_{N-2,0}^{(\alpha)} & \cdots & w_{2,0}^{(\alpha)} & w_{1,0}^{(\alpha)} & w_{0,0}^{(\alpha)} \end{pmatrix},$$

and

$$A_{-1,2} = \frac{1}{h^\alpha}\begin{pmatrix} 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ w_{0,-1}^{(\alpha)} & 0 & 0 & 0 & \cdots & 0 & 0 \\ w_{1,-1}^{(\alpha)} & w_{0,-1}^{(\alpha)} & 0 & 0 & \ddots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & 0 & \vdots \\ w_{N-4,-1}^{(\alpha)} & w_{N-5,-1}^{(\alpha)} & w_{N-6,-1}^{(\alpha)} & \cdots & \ddots & 0 & 0 \\ w_{N-3,-1}^{(\alpha)} & w_{N-4,-1}^{(\alpha)} & w_{N-5,-1}^{(\alpha)} & \cdots & w_{0,-1}^{(\alpha)} & 0 & 0 \\ w_{N-2,-1}^{(\alpha)} & w_{N-3,-1}^{(\alpha)} & w_{N-4,-1}^{(\alpha)} & \cdots & w_{1,-1}^{(\alpha)} & w_{0,-1}^{(\alpha)} & 0 \end{pmatrix}$$

and $A_{r,2}{}^T, r = -1, 0, 1$, denote the transposes corresponding to the right fractional derivative.

Now, let $\hat{U}^m$ be the solution of (31) without the error term and $\hat{U}^m = [\hat{u}_0^m, \hat{u}_1^m, \cdots, \hat{u}_N^m]^T$. Also, let $\hat{L}_\alpha$ and $\hat{B}_\alpha$ be matrices obtained by excluding their first and last rows and columns of L_α and B_α, respectively, and let $\hat{F}^{m+1/2}$ be the vector obtained by eliminating the first and last entries of $F^{m+1/2}$. Having imposed the boundary conditions, given by (29), on (31), we have the following ready-to-solve system:

$$(\hat{L}_\alpha - \hat{B}_\alpha)\hat{U}^{m+1} = (\hat{L}_\alpha + \hat{B}_\alpha)\hat{U}^m + \tau\hat{L}_\alpha\hat{F}^{m+1/2} + \hat{\mathbf{b}}^m \quad (32)$$

and

$$\hat{\mathbf{b}}^m = (L_\alpha + B_\alpha)_0\phi_1^m + (L_\alpha + B_\alpha)_N\phi_2^m - (L_\alpha - B_\alpha)_0\phi_1^{m+`1} - (L_\alpha - B_\alpha)_N\phi_2^{m+1},$$

$m = 0, 1, \ldots, M-1$, where the subscripts 0 and N denote the first and last columns of $\hat{L}_\alpha$ and $\hat{B}_\alpha$, respectively.

NUMERICAL TESTS AND RESULTS

We use the following example to test the performance of our proposed schemes:

Let

$$H(x,m,\alpha) = \frac{\Gamma(m+1)}{\Gamma(m+1-\alpha)}(x^{m-\alpha} + (1-x)^{m-\alpha}),$$

$$S_0(x) = x^5(1-x)^5,$$

$$K_1 = 1 = K_2,$$

$$f(x,t) = -e^t\big(S_0(x) + H(x,5,\alpha) - 5H(x,6,\alpha) + 10H(x,7,\alpha) - 10H(x,8,\alpha) + 5H(x,9,\alpha) - H(x,10,\alpha)\big)$$ and

$u(x,0) = S_0(x), u(0,t) = 0, u(1,t) = 0.$

With the above information, the exact solution of the FDE is given by

$u(x,t) = S_0(x)e^{-t}.$

We partition the computational space domain into N subintervals and the time domain into $M = N^2$ subintervals. The numerical convergence orders p_n were computed by the formula

$$p_n = \frac{\ln\left[\frac{\|E^{n-1}\|_\infty}{\|E^n\|_\infty}\right]}{\ln\left[\frac{h_{n-1}}{h_n}\right]}$$

where u denotes the exact solution and $E^n = u^n - \hat{u}^n$, h_n is the step size of the grid used for E^n and $\|E^n\|_\infty$ denotes the maximum norm.

The developed Crank-Nicolson schemes were applied to the one-dimensional space fractional diffusion equation and were tested with numerical tests. In each case, the errors were computed with respect to the infinity norm, and convergence orders were calculated by (33) with binary logarithm. The errors and convergence orders were exhibited in Table 1 and Table 2 with different space and time grid lengths leading to shifting parameters $(r_1, r_2) = (1, 0)$ and $(1, -1)$, respectively. It can be observed from the results of both the tables that the errors converge to zero as the step

Table 1: Maximum errors and convergence orders of C-N scheme: $(r_1, r_2) = (1,0)$.

h	τ	α = 1.1		α = 1.5		α = 1.9	
N	M	$\|E^n\|_\infty$	Order	$\|E^n\|_\infty$	Order	$\|E^n\|_\infty$	Order
4	16	1.0082E-05	-	7.3024E-05	-	7.6810E-05	-
8	64	1.2263E-06	3.04	4.1046E-06	4.15	2.9039E-06	4.73
16	256	1.2940E-07	3.24	1.6168E-07	4.67	9.7053E-08	4.90
32	1024	9.5701E-09	3.76	8.0170E-09	4.33	5.1823E-09	4.23
64	4096	6.4520E-10	3.89	4.5026E-10	4.15	3.0970E-10	4.06
128	16384	4.1856E-11	3.95	2.5997E-11	4.11	1.8476E-11	4.07
256	65536	2.6632E-12	3.97	1.5450E-12	4.07	1.1182E-12	4.05

Table 2: Maximum errors and convergence orders of C-N scheme: $(r_1, r_2) = (1, -1)$.

h	τ	α = 1.1		α = 1.5		α = 1.9	
N	M	$\|E^n\|_\infty$	Order	$\|E^n\|_\infty$	Order	$\|E^n\|_\infty$	Order
4	16	1.6017E-05	-	3.8292E-05	-	6.8428E-05	-
8	64	7.2285E-07	4.47	1.9971E-06	4.26	2.6187E-06	4.71
16	256	8.8343E-08	3.03	1.8344E-07	3.44	1.4221E-07	4.20
32	1024	8.6201E-09	3.36	1.3216E-08	3.80	8.5756E-09	4.05
64	40961	6.4640E-10	3.74	8.6600E-10	3.93	5.2606E-10	4.03
128	6384	4.3994E-11	3.88	5.5333E-11	3.97	3.3280E-11	3.98

size decreases, and the convergence order is near 4. Hence, the numerical results suggest that the approximations are unconditionally stable and converge with order 4 accuracy.

CONCLUSION

Two new quasi-compact fourth-order schemes for fractional derivatives were established. A C-N scheme for each approximation was formulated to obtain numerical solutions of a one-dimensional space fractional diffusion equation. Numerical results confirm the convergence and order of accuracy of the approximations established. Numerical tests also show that the schemes are unconditionally stable for any choice of space discretization. Analysis of the stability properties is open to be established.

ACKNOWLEDGEMENT

The authors sincerely thank the reviewers for their fruitful suggestions that improved the quality of manuscript and the Postgraduate Institute of Science, University of Peradeniya, for their numerous support to succeed in completing this manuscript.

DECLARATION OF CONFLICT OF INTEREST

The authors declare that no conflict of interest.

REFERENCES

Cai, M. and Li, C. (2020). Numerical approaches to fractional integrals and derivatives: A review. *Mathematics* **8**(1), 43. DOI: https://doi.org/10.3390/math8010043.

Diethelm, K. (2010). *The Analisis of Fractional Differential Equations: An Application Oriented Exposition Using Differential Operators of Caputo Type.* Springer, Science & Business Media. DOI: https://doi.org/10.1007/978-3-642-14574-2.

Gunarathna, W. A., Nasir, H. M. and Daundasekera, W. B. (2019). An exexplicitorm for higher order approximations of fractional derivatives. *Applied Numerical Mathematics* **143**: 51-60. DOI: https://doi.org/10.1016/j.apnum.2019.03.017

Hao, Z. P., Sun, Z. Z. and Cao, W. R. (2015). A fourth-order approximation of fractional derivatives with its applications. *Journal of Computational Physics* **281**: 787-808. DOI: https://doi.org/10.1016/j.jcp.2014.10.053.

Koeller, R. C. (1984). Applications of fractional calculus to the theory of viscoelasticity. *Journal of Applied Mechanics* **51**(2): 299-307. DOI: http://dx.doi.org/10.1115/1.3167616.

Lubich, C. (1986). Discretized fractional calculus. *SIAM Journal on Mathematical Analysis* **17**(3): 704-719. DOI: https://doi.org/10.1137/0517050.

Meerschaert, M. M. and Tadjeran, C. (2004). Finite difference approximations for fractional advection–dispersion flow equations. *Journal of Computational and Applied Mathematics* **172**(1): 65-77. DOI: https://doi.org/10.1016/j.cam.2004.01.033.

Metzler, R. and Klafter, J. (2004). The restaurant at the end of the random walk: recent developments in the description of anomalous transport by fractional dynamics. *Journal of Physics A: Mathematical and General* **37**(31): R161. DOI: 10.1088/0305-4470/37/31/R01.

Nasir, H. M., Gunawardana, B. K. and Abeyrathna, H. P. (2013). A second order finite difference approximation for the fractional diffusion equation. *International Journal of Applied Physics and Mathematics* **3**(4): 237-243. DOI: 10.7763/IJAPM.2013.V3.212.

Nasir, H. M. and Nafa, K. (2018a). A new second order approximation for fractional derivatives with applications. *SQU Journal of Science* **23**(1): 43-55. DOI: https://doi.org/10.24200/squjs.vol23iss1pp43-55 .

Nasir, H. M. and Nafa, K. (2018b). Algebraic construction of a third order difference approximations for fractional derivatives and applications. *ANZIAM Journal* **59**: C254-C269. https://doi.org/10.21914/anziamj.v59i0.12592 .

Podlubny, I. (1998). *Fractional Differential Equations: An Introduction to Fractional Derivatives, Fractional Differential Equations, to Methods of Their Solution and Some of Their Applications.* Elsevier. DOI: 10.4236/am.2020.1111074.

Rossikhin, Y. A., & Shitikova, M. V. (1997). Applications of fractional calculus to dynamic problems of linear and nonlinear hereditary mechanic of solids. *Appl.Mech.Rev* **50**(1): 15-67. DOI: https://doi.org/10.1115/1.3101682.

Sun, H., Zhang, Y., Baleanu, D., Chen, W., & Chen, Y. (2018).. A new collection of real world applications of fractional calculus in science and engineering. *Communication in Nonlinear Science and Numerical Simulation* **64:** 213-231. DOI: https://doi.org/10.1016/j.cnsns.2018.04.019 .

Tadjeran, C., Meerschaert, M. M. and Scheffler, H. P. (2006). A secorder accurate rate numerical approximation for the fractional diffusion equation. *Journal of Computational Physics* **213**(1): 205-213. DOI: https://doi.org/10.1016/j.jcp.2005.08.008.

Tian, W., Zhou, H. and Deng, W. (2015). A class of second order difference approximations for solving space fractional diffusion equations. *Mathematics of Computations* **84**(294): 1703-1727. DOI: https://doi.org/10.1090/S0025-5718-2015-02917-2

Zhou, H., Tian, W. and Deng, W. (2013). Quasi-compact finite difference schemes for space fractional diffusion equations. *Journal of Scientific Computing* **56**(1): 45-66. DOI: https://doi.org/10.1007/s10915-012-9661-0

Sun, H., Zhang, Y., Baleanu, D., Chen, W., & Chen, Y. (2018). A new collection of real world applications of fractional calculus in science and engineering. *Communications in Nonlinear Science and Numerical Simulation*, **64**, 213-231. DOI: https://doi.org/10.1016/j.cnsns.2018.04.019.