Algebraic construction of higher order difference approximations for fractional derivatives and applications

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A generalization of the Grünwald difference approximation for fractional derivatives in terms of a real sequence and its generating function is presented. Properties of the generating function are derived for consistency and order of accuracy for the approximation corresponding to the generator. Using this generalization, some higher order Grünwald type approximations are constructed and tested for numerical stability by using steady state fractional differential problems. These higher order approximations are used in Crank-Nicolson type numerical schemes to approximate the solution of space fractional diffusion equations. Stability and convergence of these numerical schemes are analysed and are supported by numerical examples.

Keywords: Fractional diffusion equation, Grünwald Approximation, Generating function, Crank-Nicolson scheme.

1 Introduction

Fractional calculus has a history that goes back to L’Hospital, Leibniz and Euler [8, 5]. A historical account of early works on fractional calculus can be found, for eg., in [18]. Fractional integral and fractional derivative are extensions of the integer order integrals and derivatives to a real or complex order. Various definitions of fractional derivatives have been proposed, among which the Riemann-Liouville, Grünwald-Letnikov and Caputo derivative are common and established. There are also definitions based on Laplace and Fourier transforms. Each definition characterizes certain properties of the integer order derivatives.

Recently, fractional calculus found its way into the application domain in science and engineering. The field of application includes, but not limited to, oscillation phenomena [11], visco-elasticity [1], control theory [21] and transport problem [13]. Fractional derivative is also found to be more suitable to describe anomalous transport in an external field derived from the continuous time random walk [2], resulting in a

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fractional diffusion equation (FDE). The FDE involves fractional derivative either in time, in space or in both variables.

A finite difference type approximation for fractional derivative is the Grünwald approximation obtained from the Grünwald-Letnikov definition. Numerical experience and theoretical justifications have shown that application of this approximation as it is in the space fractional diffusion equation (SFDE) results in unstable solutions when explicit, implicit and even the Crank-Nicolson (CN) schemes are used [11]. The latter two schemes are popular for their unconditional stability for classical diffusion equations with integer order derivatives. This peculiar phenomenon for the implicit and CN schemes is corrected and the stability is restored when a shifted form of the Grünwald approximation is used [11] [12].

The Grünwald approximation is known to be of first order with the space discretization size $h$ in the shifted and non-shifted form and is, therefore, useful only in first order schemes for the SFDE such as explicit Euler (forward) and implicit Euler (backward) methods. Since the CN approximation scheme is of second order in time step $\tau$, Meerschaert et al. [19] used extrapolation improvement for the space discretization to obtain a second order accuracy. Subsequently, second order approximations for the space fractional derivatives were obtained through some manipulations on the first order Grünwald approximation. Nasir et al. [14] obtained a second order accuracy through a non-integer shift in the Grünwald approximation, displaying super convergence. Convex combinations of various shifts of the shifted Grünwald approximation were used to obtain higher order approximation in Chinese schools [20, 6, 25]. Zhao and Deng [24] extended the concept of super convergence to derive a series of higher order approximations.

Earlier, Lubich [9] obtained higher order approximations for the fractional derivative for orders up to 6 with no shifts involved. Numerical experiments show that these approximations are also unstable for the SFDE when the numerical methods mentioned above are used. Shifted forms of these higher order approximations diminish the order to one, making them unusable as Chen and Deng [11] [12] observed. We give a simple proof of this observation from our main result.

The present authors generalized the concept of Grünwald difference approximation by identifying it with representing generating functions. We establish properties of this approximating generating function for consistency and order of accuracy. This generalization opens a door for more choices of Grünwald type approximations.

In this paper, we construct algebraically some higher order shifted Grünwald type approximations for the fractional derivative. Interestingly, our newly constructed approximations turn out to be shifted extension counterparts of the Lubich formula. We apply some of the approximations in the CN type schemes in FDEs with justification of stability and convergence.

The rest of the paper is organized as follows. In Section 2 definitions and notations are introduced. In Section 3 the main results of generalization is presented. In Section 4 higher order approximations with shifts are constructed with some numerical tests to select suitable approximation methods. In Section 5 some selected methods are applied to device numerical schemes for space fractional diffusion equation. Stability and convergence for the schemes are analysed in Section 6. Supporting numerical results are presented in Section 7 and conclusion are drawn in Section 8.
2 Definitions and Notations

Let $L_1(\Omega) = \{ f | \int_{-\infty}^{\infty} |f(x)| dx < \infty \}$ denote the space of Lebesgue integrable functions. The Fourier transform (FT) of $f(x) \in L_1(\mathbb{R})$ is defined by $\hat{f}(\eta) = \int_{-\infty}^{\infty} f(x)e^{-i\eta x}dx$, $\eta \in \mathbb{R}$. The inverse FT is $f(x) = \int_{-\infty}^{\infty} \hat{f}(\eta)e^{i\eta x}d\eta$. The FT is linear: for $\alpha, \beta \in \mathbb{R}$, and $f, g \in L_1(\mathbb{R})$, $\hat{f}(\alpha f + \beta g)(\eta) = \alpha \hat{f}(\eta) + \beta \hat{g}(\eta)$. For a function $f$ at a point $x \in \mathbb{R}$, the FT is given by $\hat{f}(\eta) = e^{ix\eta}f(\eta)$. For $\alpha \in \mathbb{R}$, denote $\mathcal{C}^{m+\alpha}(\mathbb{R}) = \{ f \in L_1(\mathbb{R}) | \int_{-\infty}^{\infty} (1 + |\eta|)^{\alpha} |\hat{f}(\eta)|d\eta \}$.

The left and right Grünwald-Letnikov (GL) fractional derivatives are given respectively by

\[
\begin{align*}
&-\infty D_x^\alpha f(x) = \lim_{h \to 0} \frac{1}{h^\alpha} \sum_{k=0}^{\infty} (-1)^k \binom{\alpha}{k} f(x - kh) \\
&x D_x^\alpha f(x) = \lim_{h \to 0} \frac{1}{h^\alpha} \sum_{k=0}^{\infty} (-1)^k \binom{\alpha}{k} f(x + kh)
\end{align*}
\]

where $\binom{\alpha}{k} = \frac{\Gamma(\alpha+1)}{\Gamma(\alpha-k+1)k!}$. The FT of the left and right fractional derivatives are $\hat{f}(-\infty D_x^\alpha f(x))(\eta) = (i\eta)^\alpha \hat{f}(x)$ and $\hat{f}(x D_x^\alpha f(x))(\eta) = (-i\eta)^\alpha \hat{f}(x)$ respectively [16]. For a fixed $h$, the finite difference type Grünwald approximations for the left and right fractional derivatives are obtained by simply dropping the limit in the GL definitions (1) and (2) as

\[
\begin{align*}
\delta_{-h}^\alpha f(x) &= \frac{1}{h^\alpha} \sum_{k=0}^{\infty} g_k^{(\alpha)} f(x - kh), \quad &\delta_{+h}^\alpha f(x) &= \frac{1}{h^\alpha} \sum_{k=0}^{\infty} g_k^{(\alpha)} f(x + kh),
\end{align*}
\]

where $g_k^{(\alpha)} = (-1)^k \binom{\alpha}{k}$ are the coefficients of the Taylor series expansion of the generating function $(1 - z)^\alpha$. These coefficients can be computed by the recursive formula $g_0^{(\alpha)} = 1$, $g_k^{(\alpha)} = (1 - \frac{\alpha+1}{k}) g_{k-1}^{(\alpha)}$, $k = 1, 2, 3, \ldots$, and satisfy the properties $g_1^{(\alpha)} = -\alpha \leq 0$, $\sum_{k=0}^{\infty} g_k^{(\alpha)} = 0$, $\sum_{k=0}^{M} g_k^{(\alpha)} \leq 0$, $\forall M \geq 2$.

When $f(x)$ is defined in the intervals $[a, b]$, it is zero-extended outside the interval to adopt these definitions of fractional derivatives and their approximations. The sums are restricted to finite up to $N$ which grows to infinity as $h \to 0$. Often, $N$ is chosen to be $N = \left[ \frac{x-a}{h} \right]$ and $N = \left[ \frac{b-x}{h} \right]$ for the left and right fractional derivatives respectively to cover the sum up to the boundary of these domain intervals, where $[y]$ is the integer part of $y$. The left and right fractional derivatives, in this case, are denoted by $aD_x^\alpha$ and $xD_x^\alpha$ respectively.

The Grünwald approximations are of first order accuracy and display unstable solutions in the approximation of SFDE by implicit and CN type schemes [11]. As a remedy, shifted forms of left and right Grünwald formulas with shift $r$ are used:

\[
\delta_{x+h}^{\alpha+\tau} f(x) = \frac{1}{h^\alpha} \sum_{k=0}^{N+r} g_k^{(\alpha)} f(x + (k - r)h), \quad x > a,
\]

where $N = \left[ \frac{x-a}{h} \right]$ or $N = \left[ \frac{b-x}{h} \right]$ for left and right fractional derivatives respectively and the upper limits of the summations have been adjusted to cover the shift $r$. 

\[3\]
Meerchaert et al. [11] showed that for a shift \( r = 1 \), the \( \delta_{x,h,1}^\alpha f(x) \) are again of first order approximations with unconditional stability restored in implicit and CN type schemes for SFDEs.

For higher order approximations, Nasir et al. [14] derived a second order approximation by a non-integer shift, displaying super convergence.

\[
\delta_{-h,\alpha/2} f(x) = a D_x^\alpha f(x) + O(h^2). \tag{5}
\]

Chen et al. [20] used convex combinations of different shifted Grünwald forms to obtain two order 2 approximations.

\[
\lambda_1 \delta_{-h,p} + \lambda_2 \delta_{-h,q} = a D_x^\alpha f(x) + O(h^2), \quad \lambda_1 + \lambda_2 = 1 \tag{6}
\]

with \( \lambda_1 = \frac{\alpha - 2q}{2(p-q)} \) and \( \lambda_2 = \frac{2p - \alpha}{2(p-q)} \) for \((p, q) = (1, 0), (1, -1)\). In the above, we stated the form for left fractional derivative only and analogous forms for right FD hold.

Hao et al. [6] obtained a quasi-compact order 4 approximation by incorporating the second order term in the fractional derivative. All the above approximations were derived from the fundamental GL approximation with coefficients \( g_k(\alpha) \) of the generating function \((1 - z)^\alpha\).

Higher order approximations were also obtained earlier by Lubich [9] establishing a connection with the characteristic polynomials of multistep methods for ordinary differential equations. Specifically, if \( \rho(z), \sigma(z) \) are, the characteristic polynomials of a multistep method of convergence order \( p \) [4], then \((\frac{\sigma(1/z)}{\rho(1/z)})^\alpha \) gives the coefficients for the Grünwald type approximation of same order for the fractional derivative of order \( \alpha \). From the backward multistep methods, Lubich [9] derived approximations of orders up to order six in the form \( L_p(z) = (\sum_{j=1}^{p} \frac{1}{j} (1-z)^j)^\alpha \). The generating functions \( L_p(z) \) given in Table 1 are of order \( p \) for \( 1 \leq p \leq 6 \) for the non-shift Grünwald type approximations.

| \( L_1(z) = (1 - z)^\alpha \) |
| \( L_2(z) = (\frac{1}{2} - 2z + \frac{1}{2}z^2)^\alpha \) |
| \( L_3(z) = (\frac{1}{3} - 3z + \frac{3}{2}z^2 - \frac{1}{3}z^3)^\alpha \) |
| \( L_4(z) = (\frac{1}{4} - 4z + 3z^2 - \frac{4}{3}z^3 + \frac{1}{4}z^4)^\alpha \) |
| \( L_5(z) = (\frac{1}{5} - 5z + 5z^2 - \frac{10}{3}z^3 + \frac{5}{2}z^4 - \frac{1}{5}z^5)^\alpha \) |
| \( L_6(z) = (\frac{1}{6} - 6z + \frac{15}{2}z^2 - \frac{20}{3}z^3 + \frac{15}{4}z^4 - \frac{6}{5}z^5 + \frac{1}{6}z^6)^\alpha \) |

**Table 1:** Lubich approximation generating functions

As noted for the non-shifted Grünwald approximation, these higher order approximations also display unstable solutions with implicit Euler and CN type schemes. Moreover, The shifted form of these approximations suffer the orders dropping to one and hence uninteresting.

### 3 Higher order shifted approximations

In this section, we present the generalization of the Grünwald approximation established in [13] with important results are given with proof for completion.

For a function \( f(x) \), denote the left and right Grünwald type operator with shift \( r \) and weights \( w_{k,r}^{(\alpha)} \), respectively, as

\[
\Delta_{x,h,r}^\alpha f(x) = \frac{1}{h^\alpha} \sum_{k=0}^{\infty} w_{k,r}^{(\alpha)} f(x \equiv (k - r)h). \tag{7}
\]
Definition 1. A sequence \( \{w_{k,r}^{(α)}\} \) of real numbers is said to approximate the fractional derivatives \( -∞D_x^α f(x) \) and \( zD_∞^α f(x) \) at \( x \) with shift \( r \) in the sense of Grünwald if
\[
-∞D_x^α f(x) = \lim_{h \to 0} \Delta^α_{-h,r} f(x), \quad zD_∞^α f(x) = \lim_{h \to 0} \Delta^α_{+h,r} f(x).
\]

Definition 2. A sequence \( \{w_{k,r}^{(α)}\} \) of real numbers is said to approximate the fractional derivatives \( -∞D_x^α f(x) \) and \( zD_∞^α f(x) \) with shift \( r \) and order \( p \geq 1 \) if
\[
-∞D_x^α f(x) = \Delta^α_{-h,r} f(x) + O(h^p), \quad zD_∞^α f(x) = \Delta^α_{+h,r} f(x) + O(h^p).
\] (8)

We denote the generating function of the coefficients \( w_{k,r}^{(α)} \) as
\[
W(z) = \sum_{k=0}^{∞} w_{k,r}^{(α)} z^k.
\]

An equivalent characterization of the generator \( W(z) \) for an approximation of fractional differential operator with order \( p \geq 1 \) and shift \( r \) is given by

Theorem 1. Let \( n-1 < α \leq n, m \) be a non-negative integer, \( f(x) \in C^{m+n+1}(\mathbb{R}) \) and \( -∞D_x^k f(x), zD_∞^k f(x) \in L^1(\mathbb{R}) \) for \( 0 \leq k \leq m + n + 1 \). Then, the generating function \( W(z) \) of a real sequence \( \{w_{k,r}^{(α)}\} \) approximates the left and right fractional differential operators for \( f(x) \) with order \( p \) and shift \( r \), \( 1 \leq p \leq m \), if and only if
\[
G_r(z) := \frac{1}{z^α} W(e^{-z})e^{rz} = 1 + O(z^p). \quad (9)
\]

Moreover, if \( G_r(z) = 1 + \sum_{l=p}^{∞} a_l(r)z^l \), then we have for the left fractional derivative
\[
\Delta^α_{-h,r} f(x) = -∞D_x^α f(x) + h^p a_p(r) -∞D_x^{p+α} f(x) + \cdots + O(h^m), \quad (10)
\]
\[
\Delta^α_{+h,r} f(x) = zD_∞^α f(x) + h^p a_p(r) zD_∞^{p+α} f(x) + \cdots + O(h^m) \quad (11)
\]

Proof. We prove the result for the left fractional derivative. Taking FT of \( \Delta^α_{h+r} f(x) \) in (7), with the help of linearity, we obtain
\[
\mathcal{F}(\Delta^α_{h,r} f(x))(η) = \frac{1}{h^α} \sum_{k=0}^{∞} w_{k,r}^{(α)} \mathcal{F}(f(x - (k - r)h))(η)
\]
\[
= \frac{1}{h^α} \sum_{k=0}^{∞} w_{k,r}^{(α)} e^{-(k-r)ihη} \hat{f}(η)
\]
\[
= \frac{e^{rzh}}{(ih)^α} \sum_{k=0}^{∞} w_{k,r}^{(α)} e^{-kzh}(iη)^α \hat{f}(η)
\]
\[
= \frac{e^{rzh}}{z^α} \left[ \sum_{k=0}^{∞} w_{k,r}(e^{-z})^k \right] (iη)^α \hat{f}(η)
\]
\[
= \frac{e^{rzh}}{z^α} W(e^{-z})(iη)^α \hat{f}(η) = G_r(z)(iη)^α \hat{f}(η)
\]
\[
= \sum_{l=0}^{∞} a_l(r)z^l(iη)^α \hat{f}(η) = \sum_{l=0}^{∞} a_l(r)h^l(iη)^{l+α} \hat{f}(η),
\]
where we have used $z = i\eta h$. Applying inverse FT, we have

$$\Delta_{h,r}^{\alpha} f(x) = \sum_{l=0}^{m-1} a_l(r) a^{l+\alpha} f(x)h^l + O(h^m). \quad (12)$$

Now, (9) holds if and only if $a_0(r) = 1, a_l(r) = 0$, for $l = 1, 2, \ldots, p - 1$. Moreover, (10) holds from (12) with (9).

One of the consequence of Theorem 1 is the following consistency condition.

**Corollary 1.** If the generating function $W(z)$ gives a consistent approximation of the left and right fractional differential operator, then the following hold:

1. $W(1) = 0$,
2. $\sum_{k=0}^\infty w_{k,r}^{(\alpha)} = 0$,
3. The fractional derivative of constant is zero.

**Proof.**

1. Since the order $p$ is at least one, when $h \neq 0$, and hence $z \neq 0$, the condition (9) becomes $W(e^{-z})e^{\pm rz} = z^\alpha(1 + O(z^p))$. Take limit as $h \to 0(z \to 0)$.
2. follows immediately with (9) and 3. If $f(x) = C$, then (7) gives $\Delta_{h,r} C = C' \sum_{k=0}^\infty w_{k,r}^{(\alpha)} = 0$ and so are their limits as $h \to 0$.

Using Theorem 1 one can easily check algebraically the following propositions for the generating function of approximation operators known previously in [14, 20, 9, 4].

**Proposition 1.** The approximation given by (5) is of second order accuracy.

**Proof.** The coefficients $g_k^{(\alpha)}$ have the generating function $(1 - z)^{\alpha}$. Since the shift of the approximation is $r = \alpha/2$, it is enough to check the function $G(z) = \frac{1}{z}\alpha e^{\alpha/2}(1 - e^{-z})^{\alpha}$.

Taylor series expansion gives that $G(z) = 1 + \alpha^2/24z^2 + O(z^4)$ which confirms the second order.

**Proposition 2.** The approximation given by (6) is of second order accuracy.

**Proof.** Since $\delta_{-h,p}$ and $\delta_{-h,q}$ have the same generating function $(1 - z)^{\alpha}$ with shifts $p$ and $q$ respectively, The Taylor series of $G(z) = \frac{\alpha}{2}\alpha e^{\alpha/2}(1 - e^{-z})^{\alpha}$ which gives $G(z) = 1 + (-\alpha^2/6 + \alpha^2/4 + \alpha^2/2 + \alpha^2)z^2 + O(z^3)$. The coefficient of $z^2$ is non-zero for all integer shifts $p$ and $q$.

**Proposition 3.** The Lubich generating functions $W_p(z), p = 1, 2, \ldots, 6$, in Table 1 are of order $p$ accurate without shift. Moreover, if a non-zero shift $r$ is introduced to the approximation, the order reduces to one.

**Proof.** When there is no shift ($r = 0$), Taylor series expansion gives $W_p(e^{-z})/z^\alpha = 1 + O(h^p)$. When a shift $r \neq 0$ is introduced to $W_p(z)$, the order is determined by

$$e^{rz}W_p(e^{-z})/z^\alpha = (1 + O(z))(1 + O(z^p)) = 1 + O(z), \text{ for } 1 \leq p \leq 6$$

reducing the order to 1.
4 Construction of higher order approximations

We construct generating functions for higher order approximation with shifts by the use of Theorem 1 and its. The importance of Theorem 1 is that the construction process is entirely confined to algebraic manipulation with the aid of Taylor series expansion.

Theorem 1 opens a door to choose a variety of forms for generating functions for \( W(z) \). In this paper, we choose the form

\[
W(z) = (\beta_0 + \beta_1 z + \beta_2 z^2 + \cdots + \beta_p z^p)^{\alpha}
\]

(13)
to construct generators.

We have the following consistency condition for the coefficients \( u_k \), \( k \geq 0 \).

**Theorem 2.** If the generating function \( W(z) \) in (13) approximates the fractional derivative, then

\[
\beta_0 + \beta_1 + \beta_2 + \cdots + \beta_p = 0
\]

**Proof.** Using Corollary 1(1).

Generating function of the approximation of order \( p \) with shift \( r \) can be algebraically constructed by the following algorithm.

1. Set \( W(z) = (\beta_0 + \beta_1 z + \beta_2 z^2 + \cdots + \beta_p z^p)^{\alpha} \), where the coefficients \( \beta_i \) are to be determined.

2. Expand \( G(z) = \frac{W(e^{-z})e^{rz}}{z^p} \) in Taylor series:

\[
G(z) = a_0 + a_1 z + \cdots + a_l z^l + \cdots ,
\]

(14)

where \( a_l \equiv a_l(\beta, r, \alpha) \).

3. Form the system of equations by imposing order conditions

\[
a_0 = 1, \quad a_l = 0 \quad \text{for} \quad l = 1, 2, 3, \cdots, p - 1.
\]

4. Solve the systems for \( \beta_i, \quad i = 0, 1, \cdots, p \) with the additional consistency condition \( \beta_0 + \beta_1 + \cdots + \beta_p = 0 \).

We have obtained approximating generating functions \( W_{p,r}(z) \) with order \( p \), shift \( r \) for \( 1 \leq p \leq 6 \) listed in Table 2.

Note that when there is no shift, i.e., \( r = 0 \), these generating functions reduces to those in Table 1 obtained by Lubich [9].

The Grünwald weights \( u_k^{(\alpha)} \) can be computed by a recurrence formula [17, 22]. It seems that, despite higher order of approximation of \( W_{p,r}(z) \), the stability of solutions using these approximations to FDEs remains an issue. Our numerical tests on some steady state problems show that the second order approximation \( W_{2,1}(z) \) displays stability for values of \( \alpha \) in the interval \([1, 2]\). However, for the other higher order approximations, the stability is limited to a subset \([\alpha_0, 2]\), \( 1 < \alpha_0 \), of the interval \([1, 2]\). This phenomenon warrants an investigation for approximations of orders three and above.

From now on, we focus our attention on the second order approximation \( W_{2,r}(z) \). We denote the approximation operators corresponding to the generators \( W_{p,r}(z) \) by \( \Delta_{p,\pm r} \) for left and right fractional differential operators.

7
The second order approximations of generator $W$

Another approach to construct higher order approximation generators $W(z)$ is to retain the non-zero coefficient $a_2(r)$ in (13) of step 2 of the algorithm without imposing the vanishing condition. That is, one imposes conditions $a_0(r) = 1, a_l(r) = 0$ for $l = 1, 3, 4, \cdots, p$ for order $p$. This technique is similar to the method used in [25].

Then we have

$$G_r(z) = 1 + a_2(r)z^2 + O(z^p).$$
Equation (12) then gives
\[ \Delta_{p,rr}^\alpha u(x) = -\infty D_x^\alpha u(x) + a_2(r) h^2 \Delta_{x,x}^\beta u(x) + O(h^\rho) \]
\[ = -\infty D_x^\alpha u(x) + a_2(r) h^2 D^2 -\infty D_x^\alpha u(x) + O(h^\rho) \]
\[ = P_x -\infty D_x^\alpha u(x) + O(h^\rho), \]
where
\[ P_x = (I + h^2 a_2(r) D^2), \]
with \( D^2 = d^2/dx^2 \) and the identity operator \( I \).

The differential operator \( D^2 \) is approximated by the second order central difference operator \( \delta_n^2 \) given by
\[ \delta_n^2 u(x) = \frac{1}{h} (u(x-h) - 2u(x) + u(x+h)) \]
with \( \delta_n^2 u(x) = D^2 u(x) + O(h^2) \).

From this, an approximation for the operator \( P_x \) is obtained as
\[ P_h u(x) = (1 + a_2(r) h^2 \delta_n^2) u(x) \quad (17) \]
with order 4 accuracy,
\[ P_h u(x) = P_x u(x) + O(h^4). \]

Hao et al. [6] derived a fourth order approximation from the first order Grünwald approximation (4) by considering a convex combination of three of its shifted forms with an appropriate \( P_x \) and called it a quasi-compact approximation. YanYan Yu et al. [23] used this technique to derive third order schemes for tempered fractional diffusion equations. In those papers, the approximation schemes were derived directly from the first order Grünwald approximation \( (1 - z)^\alpha \).

We use the properties of general generating functions of approximations to derive higher order schemes as it allows various choices with only algebraic manipulations.
We obtained a third order quasi-compact approximation from the second order approximation generator \( W_{2,r}(z) \) without additional vanishing conditions as
\[ \Delta_{2,r}^\alpha u(x) = P_x -\infty D_x^\alpha u(x) + O(h^3), \quad (18) \]
with
\[ a_2(r) = -\frac{\alpha}{3} + r - \frac{r^2}{2\alpha}. \]

4.1 Numerical tests
We test the approximation operators of orders 2 and 3 derived in this section applying them to the steady state problem
\[ D_x^\alpha u(x) = f(x), \quad a \leq x \leq b, \quad (19) \]
\[ u(a) = \phi_0, \quad u(b) = \phi_1. \]
We briefly describe the approximation schemes for the steady state problem.
For a uniform partition \( a = x_0 < x_1 < x_2 < \cdots < x_N = b \) of the domain \([a, b] \) with subinterval size \( h \), problem (19) at \( x_i \) is approximated by the operator \( \Delta_{2,1} \). Then one gets from (15),

\[
\Delta_{2,1} u_i = f_i + O(h^2), \quad i = 0, 1, 2, \cdots N,
\]

where \( u_i = u(x_i) \) and \( f_i = f(x_i), i = 0, 1, 2, \cdots, N - 1 \). Neglecting the \( O(h^2) \) remainder term, we get the approximation scheme

\[
\Delta_{h,1} u_i = f_i, \quad i = 0, 1, 2, \cdots N, \tag{20}
\]

where \( \hat{u}_i \) the approximation of the exact solution \( u_i \) for \( i = 0, 1, 2, \cdots, N - 1 \) with \( \hat{u}_0 = \phi_0, \hat{u}_N = \phi_1 \).

Let \( U = [u_0, \hat{u}_1, \hat{u}_2, \cdots, \hat{u}_{N-1}, u_N]^T, \quad F = [f_0, f_1, f_2, \cdots, f_N]^T \) with the boundary conditions incorporated in \( U \). Then, the matrix formulation of (20) is given by \( A_{2,1} U = F \), where \( A_{2,1} \) is an \((N + 1) \times (N + 1)\) toepilz matrix given by

\[
A_{2,1}(i, j) = \begin{cases} w^{(a)}_{i-j+1,1}, & i \geq j - 1 \\ 0, & \text{elsewhere.} \end{cases}
\]

Bringing the boundary values to the right side, the reduced system becomes,

\[
\hat{A}_{2,1} \hat{U} = \hat{F} - A_0 \phi_0 - A_N \phi_1, \tag{21}
\]

where \( \hat{A}_{2,1} \) is the reduced matrix obtained from \( A_{2,1} \) by deleting the first and last rows and columns, \( \hat{U}, \hat{F} \) are obtained from \( U, F \) respectively by deleting their first and last boundary entries. \( A_0, A_N \) are the first and last column vectors of the matrix \( A_{2,1} \) reduced at both ends as above. The approximate solution is then obtained by solving the matrix equation (21).

For the right fractional derivative \( D_x^\alpha u(x) \), the approximation matrix is given by \( A_{2,1}^T \).

We derive a third order quasi-compact approximation as follows. We pre-multiply (19) by the operator \( P_x \).

\[
P_x a D_x^\alpha u(x) = P_x f(x), \quad a \leq x \leq b.
\]

From (18), the operator \( P_x a D_x^\alpha \) is approximated by \( \Delta_{2,1} \) with order 3. At the grid point \( x_i \), we get

\[
\Delta_{2,1} u_i = P_h f_i + O(h^3), \quad i = 0, 1, 2, \cdots N,
\]

where \( P_h \) is given in (17).

It is expressed in matrix form as \( A_{2,1} U = PF \), where \( P \) is the matrix corresponding to \( P_h \) and given by the tri-diagonal matrix

\[
P = Tri[a_2(1), 1 - 2h^2 a_2(1), a_2(1)]. \tag{22}
\]

After imposing boundary conditions, we obtain the ready-to-solve third order scheme as

\[
\hat{A}_{2,1} \hat{U} = \hat{P} \hat{F} - A_0 \phi_0 - A_N \phi_1, \tag{23}
\]

where \( \hat{P} \) is the reduced matrix of \( P \).

Note that we have the same approximation operator \( \Delta_{2,1} \) for both approximations of orders 2 and 3 and hence have the same matrix \( A_{2,1} \). The pre-multiplication of
$P_x$ improves the order of accuracy from 2 to 3. We prefer to call the operator $P_x$ a preconditioner to the fractional differential operator.

We test the approximation scheme devised in this subsection using the steady state test problem

$$0D_x^a u(x) = \frac{10\Gamma(n + 1)}{\Gamma(n + 1 - \alpha)} x^{n-\alpha}, \quad 0 \leq x \leq 1,$$

$$u(0) = 0, \quad u(1) = 10$$

with the exact solution $u(x) = 10x^n$. We set $n = 8$ and test for various values of the parameter $\alpha$. First, we test the second order approximation (21) with $\alpha = 1.1, 1.5$ and $1.9$. The number of grid subintervals $N$ corresponding to the discretization size $h = (1 - 0)/N$ was considered for values $N = 16, 32, \ldots, 1024$. The maximum error $\|u - U\|_\infty$ and the computed convergence orders are listed in Table 3.

| $N$ | $\|u - U\|_\infty$ | $\alpha = 1.1$ Order | $\|u - U\|_\infty$ | $\alpha = 1.5$ Order | $\|u - U\|_\infty$ | $\alpha = 1.9$ Order |
|-----|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 16  | 4.8893e-01      | ~               | 2.5141e-01      | ~               | 1.3365e-01      | ~               |
| 32  | 1.1592e-01      | 2.08            | 6.4851e-02      | 1.95            | 3.3951e-02      | 1.98            |
| 64  | 2.7227e-02      | 2.09            | 1.6450e-02      | 1.98            | 8.5491e-03      | 1.99            |
| 128 | 6.3685e-03      | 2.10            | 4.1396e-03      | 1.99            | 2.1446e-03      | 2.00            |
| 256 | 1.4873e-03      | 2.10            | 1.0383e-03      | 2.00            | 5.3703e-04      | 2.00            |
| 512 | 3.5020e-04      | 2.09            | 2.5997e-04      | 2.00            | 1.3437e-04      | 2.00            |
| 1024| 8.7574e-05      | 2.00            | 6.5044e-05      | 2.00            | 3.3606e-05      | 2.00            |

Table 3: Second order Approximation with shift $r = 1$ using $W_{2,r}$

Next, we test the order 3 quasi-compact approximation (23) with the same setting of parameters used for the previous testing. The test results are given in Table 4. These tests confirm the theoretical justifications of the orders of the two schemes.

| $N$ | $\|u - U\|_\infty$ | $\alpha = 1.1$ Order | $\|u - U\|_\infty$ | $\alpha = 1.5$ Order | $\|u - U\|_\infty$ | $\alpha = 1.9$ Order |
|-----|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 16  | 9.8696e-03      | ~               | 1.3027e-02      | ~               | 3.8208e-03      | ~               |
| 32  | 1.0719e-03      | 3.15            | 1.6435e-03      | 3.00            | 4.6147e-04      | 3.03            |
| 64  | 1.2038e-04      | 3.13            | 2.0611e-04      | 3.00            | 5.6560e-05      | 3.01            |
| 128 | 1.3765e-05      | 3.11            | 2.5805e-05      | 3.00            | 7.0003e-06      | 3.01            |
| 256 | 1.5891e-06      | 3.11            | 3.2281e-06      | 3.00            | 8.7069e-07      | 3.00            |
| 512 | 1.8439e-07      | 3.01            | 4.0366e-07      | 3.00            | 1.0857e-07      | 3.00            |
| 1024| 2.2872e-08      | 3.00            | 5.0467e-08      | 3.00            | 1.3563e-08      | 2.96            |

Table 4: Third order Approximation with shift $r = 1$ using $W_{2,1}$

5 Approximation of fractional diffusion equation

We apply the approximations constructed in the previous section to the numerical approximation of the space fractional diffusion equation defined in the domain $[a, b] \times [0, T]$:

$$\frac{\partial u(x, t)}{\partial t} = K_1 aD_x^a u(x, t) + K_2 xD_x^b u(x, t) + f(x, t),$$

(24)
with the initial and boundary conditions

\[
\begin{align*}
    u(x, 0) &= s_0(x), & x \in [a, b] \\
    u(a, t) &= \phi_1(t), \ u(b, t) = \phi_2(t), & t \in [0, T],
\end{align*}
\]

where \( u(x, t) \) is the unknown function to be determined; \( K_1, K_2 \) are non-negative constant diffusion coefficients with \( K_1 + K_2 \neq 0 \), i.e., not both are simultaneously zero, and \( f(x, t) \) is a known source term. The boundary conditions are set as follows: If \( K_1 \neq 0 \), then \( \phi_1(t) \equiv 0 \) and if \( K_2 \neq 0 \), then \( \phi_2(t) \equiv 0 \). We assume that the diffusion problem has a unique solution.

The space domain \([a, b]\) is partitioned into a uniform mesh of size \( N \) with subintervals of length \( h = (b - a)/N \), and the time domain \([0, T]\) into a uniform partition of size \( M \) with subintervals of length \( \tau = T/M \). These two partitions form a uniform partition of the 2-D domain \([a, b] \times [0, T]\) with grid points \((x_i, t_m)\), where \( x_i = a + ih \) and \( t_m = m\tau \), \( 0 \leq i \leq N, \ 0 \leq m \leq M \). We use the following notations for conciseness: \( u_i^m = u(x_i, t_m) \), \( t_{m+1/2} = \frac{1}{2}(t_{m+1} + t_m) \) and \( f_i^{m+1/2} = f(x_i, t_{m+1/2}) \).

We present the CN type scheme with the third order approximation in (18) for the \( \frac{\partial^2 u}{\partial x^2} \) with the initial and boundary conditions

\[
\begin{align*}
    u(x, 0) &= s_0(x), & x \in [a, b] \\
    u(a, t) &= \phi_1(t), \ u(b, t) = \phi_2(t), & t \in [0, T],
\end{align*}
\]

where \( u(x, t) \) is the unknown function to be determined; \( K_1, K_2 \) are non-negative constant diffusion coefficients with \( K_1 + K_2 \neq 0 \), i.e., not both are simultaneously zero, and \( f(x, t) \) is a known source term. The boundary conditions are set as follows: If \( K_1 \neq 0 \), then \( \phi_1(t) \equiv 0 \) and if \( K_2 \neq 0 \), then \( \phi_2(t) \equiv 0 \). We assume that the diffusion problem has a unique solution.

The space domain \([a, b]\) is partitioned into a uniform mesh of size \( N \) with subintervals of length \( h = (b - a)/N \), and the time domain \([0, T]\) into a uniform partition of size \( M \) with subintervals of length \( \tau = T/M \). These two partitions form a uniform partition of the 2-D domain \([a, b] \times [0, T]\) with grid points \((x_i, t_m)\), where \( x_i = a + ih \) and \( t_m = m\tau \), \( 0 \leq i \leq N, \ 0 \leq m \leq M \). We use the following notations for conciseness: \( u_i^m = u(x_i, t_m) \), \( t_{m+1/2} = \frac{1}{2}(t_{m+1} + t_m) \) and \( f_i^{m+1/2} = f(x_i, t_{m+1/2}) \).

We present the CN type scheme with the third order approximation in (18) for the space fractional derivative using \( W_{2,1}(z) \) with the preconditioner operator \( P_x = 1 + h^2a_2(1)D^2 \). For the second order approximation in (15), \( P_x \) will be the unit operator \( I \).

Preconditioning (24) by \( P_x \), one gets the equivalent equation

\[
P_x \delta_t u(x, t) = D u(x, t) + P_x f(x, t),
\]

where \( D = K_1 P_x aD_x^\alpha + K_2 P_x xD_x^\alpha \).

Using the approximations \( \Delta_2 = K_1 \Delta_{2,+,1} + K_2 \Delta_{2,-1} \) of order 3 for \( D \), \( P_h \) of order 4 for \( P \), and the second order approximations

\[
\frac{\partial u(x, t)}{\partial t} = \frac{u(x, t + \tau) - u(x, t)}{\tau} + O(\tau^2) \quad \text{and} \quad u(x, t + \tau/2) = \frac{u(x, t + \tau) + u(x, t)}{2} + O(\tau^2),
\]

the Crank-Nicolson type scheme at \((x_i, t_m), 0 \leq i \leq N - 1, 0 \leq m \leq M \), is given by

\[
P_h \frac{u_i^{m+1} - u_i^m}{\tau} = \Delta_2 \left( u_i^{m+1} + u_i^m \right) + P_h f_i^{m+1/2} + O(\tau^2 + h^p), \quad p = 2, 3. \tag{25}
\]

Here, \( P_h = I \) for \( p = 2 \).

Let \( U^m \) be the solution of (25) after neglecting the \( O(\tau^2 + h^p) \) terms with \( U^m = [\hat{u}_0^m, \hat{u}_1^m, \hat{u}_2^m, \ldots, \hat{u}_{N-1}^m, \hat{u}_N^m]^T \), where \( \hat{u}_i^m \) becomes the approximation of the exact values \( u_i^m \). Then, (25) becomes

\[
P_h (\hat{u}_i^{m+1} - \hat{u}_i^m) = \frac{\tau}{2} \Delta_2 (\hat{u}_i^{m+1} + \hat{u}_i^m) + \tau P_h f_i^{m+1/2}, 0 \leq i \leq N, 0 \leq m \leq M - 1.
\]

Thus, the Crank-Nicolson type scheme in matrix form reads

\[
P (U^{m+1} - U^m) = B (U^{m+1} + U^m) + \tau PF^{m+1/2}, 0 \leq m \leq M - 1, \tag{26}
\]

where \( F^{m+1/2} = \tau [f_1^{m+1/2}, f_2^{m+1/2}, \ldots, f_{N}^{m+1/2}]^T \), \( P \) is given in (22). The matrix \( B \) is corresponding to the operator \( \Delta_2 \) given by \( B = \frac{\tau}{2} (K_1 A_{2,1} + K_2 A_{2,1}^T) \). Re-arranging for \( U^{m+1} \) and \( U^m \), we have

\[
(P - B)U^{m+1} = (P + B)U^m + \tau PF^{m+1/2}, \quad m = 0, 1, 2, \ldots, M - 1. \tag{27}
\]
Let \( \hat{P} \) and \( \hat{B} \) be the reduced matrix from \( P \) and \( B \) respectively, and \( \hat{F}^{m+1/2} \) be the reduced vector from \( F^{m+1/2} \) as was in Section 4.1.

After imposing the boundary conditions, equation (27) reduces to the ready-to-solve form

\[
(\hat{P} - \hat{B})\hat{U}^{m+1} = (\hat{P} + \hat{B})\hat{U}^m + \tau\hat{P}\hat{F}^{m+1/2} + \hat{b}^m, \quad m = 0, 1, 2, \cdots, M - 1,
\]

where \( \hat{b}^m = B_0(u_{N+1}^m + u_0^m) + B_N(u_N^{m+1} + u_N^m) \) and \( B_0, B_N \) are the first(0th) and last(\( N^{th} \)) column vectors of the matrix \( B \) reduced again as before.

## 6 Stability and convergence

We establish the stability of the Crank-Nicolson scheme (27) for the approximations of orders 2 and 3 given in (15) and (18).

We closely follow the analysis in [6] and present some required results.

Let \( V_h = \{ \psi \in \mathbb{R} \} \) be the space of grid functions in the computational domain in space interval \([a, b]\).

For any \( u, v \in V_h \), define the discrete inner products and corresponding norms as

\[
(u, v) = h \sum_{i=1}^{N-1} u_i v_i,
\]

\[
\|u\| = \sqrt{(u, u)},
\]

\[
\|u\|_1 = \sqrt{\langle \delta_h u, \delta_h u \rangle}.
\]

Then, we have the following:

**Lemma 1.**

1. The operator \( P_h \) is self-adjoint.

2. The quadratic form \( (P_h u, u) \) satisfies \( \frac{1}{12} \|u\| < (P_h u, u) \leq \|u\| \) and hence the norm \( \|u\|_P = (P_h u, u) \) is equivalent to \( \|u\| \).

**Proof.** 1. \( (P_h u, v) = ((1 + h^2a_2(1)\delta_h^2)u, v) = (u, v) + h^2a_2(1)(\delta_h^2 u, v) = (u, v) - h^2a_2(1)(\delta_h u, \delta_h v) = (u, v) + h^2a_2(1)(u, \delta_h^2 v) = (u, P_h v). \)

2. For \( 1 \leq \alpha \leq 2 \), we easily see that \( \frac{1}{12} \leq a_2(1) \leq 1 - \frac{\sqrt{5}}{3} < \frac{1}{5} \). Also,\[\|u\|_2^2 = \langle \delta_h u, \delta_h u \rangle = \langle \delta_h u, \delta_h u \rangle = \langle \delta_h u, \delta_h u \rangle = \langle \delta_h u, \delta_h u \rangle \]

\[\|u\|_2^2 \leq \|\delta_h^2 u\| \|u\| \leq \|u\| \sum_{i=1}^{N-1} (u_i + 1 - 2u_i + u_{i-1}) \|u\| \leq \frac{4}{N} \|u\|^2.\]

Now, \( (P_h u, u) = (u, u) + h^2a_2(1)(\delta_h^2 u, u) = \|u\|^2 - h^2a_2(1)|u|_2^2 \leq \|u\|^2. \)

Also, \( (P_h u, u) = \|u\|^2 - h^2a_2(1)|u|_2^2 > \|u\|^2 - \frac{4}{5} \|u\|^2 = \frac{1}{5} \|u\|^2. \) Thus, the equivalence of the norm follows. \( \Box \)

**Lemma 2.** Let \( \{t_k\}_{k=0}^\infty \) be a double sided real sequence such that \((i) t_k + t_{-k} \geq 0 \) for \( k \neq 0 \), \((ii) \sum_{j=-N}^{N} t_j \leq 0 \) for \( N \geq 0 \). Then, the toeplitz matrices \( T_N = [t_{i-j}] \) of size \( N + 1 \) are negative definite for \( N \geq 0 \).

**Proof.** For \( N = 0, t_0 \leq 0 \). This matrix of size 1 is negative definite. For any positive integer \( N \) and for any \( (N + 1) \)-dimensional non-zero vector \( v = [v_0, v_1, v_2, \cdots, v_N]^T \),
consider the quadratic form $v^T T v = \sum_{i=0}^{N} \sum_{j=0}^{N} t_{j-i} v_i v_j$. Summing the terms diagonally, we have

$$v^T T_N v = \sum_{k=-N}^{N} t_k \sum_{j=0}^{N-1-k} v_j v_{k+j}$$

$$= t_0 \sum_{j=0}^{N} v_j^2 + \sum_{k=1}^{N} (t_k + t_{-k}) \sum_{j=0}^{N-1-k} v_j v_{k+j}$$

$$\leq t_0 \|v\|^2 + \sum_{k=1}^{N} (t_k + t_{-k}) \sum_{j=0}^{N-1-k} (1/2)(|v_j|^2 + |v_{k+j}|^2)$$

$$\leq t_0 \|v\|^2 + \sum_{k=1}^{N} (t_k + t_{-k}) \|v\|^2 = \sum_{k=-N}^{N} t_k \|v\|^2 \leq 0$$

\[\square\]

**Lemma 3.** The operators $\Delta_{2,1}^α$ and $\Delta_{2,-1}^α$ are self-adjoint and negative definite. Moreover, the matrices $A^α_{2,1}$ and $A^α_{2,-1}$ corresponding to the operators $\Delta_{2,1}^α$ and $\Delta_{2,-1}^α$ respectively are negative definite.

**Proof.** By virtue of Lemma 2, it is enough to prove that the coefficients $w_{k,1}$ of the generator $W_{2,1}(z) = \sum_{k=0}^{\infty} w_{k,1} z^k$ satisfy the following properties for $1 \leq \alpha \leq 2$.

$$w_{0,1} \geq 0, \quad w_{0,1} + w_{2,1} \geq 0 \quad \text{and} \quad \sum_{k=0}^{M} w_{k,1} \leq 0 \quad \text{for all} \quad M \geq 2.$$ 

Let $W_{2,1}(z) = (\beta_0 + u_1 z + \beta_2 z^2)^α$. Then, $\beta_0 = \frac{\beta_2}{\alpha} - \frac{1}{\alpha} \geq 0$, $\beta_1 = -2 - \frac{2}{\alpha} \leq 0$ and $\beta_2 = \frac{\beta_2}{\alpha} - \frac{1}{\alpha} \leq 0$ for $1 \leq \alpha \leq 2$. Also, we have $w_{0,1} = \beta_0^α \geq 0$ and $w_{1,1} = \alpha \beta_0^{\alpha-1} \beta_1 \leq 0$. Moreover,

$$w_{0,1} + w_{2,1} = \beta_0^α + \frac{1}{2} \alpha \beta_0^{\alpha-2} \left[ (\alpha - 1) \beta_1^2 + 2 \beta_0 \beta_2 \right]$$

$$= \frac{1}{2} \beta_0^{\alpha-2} \left[ \alpha (\alpha - 1) \beta_1^2 + 2 \beta_0 (\alpha \beta_2 + \beta_0) \right]$$

$$= \frac{1}{2} \beta_0^{\alpha-2} \left[ \alpha (\alpha - 1) \beta_1^2 + 2 \beta_0 \frac{(\alpha - 1)(\alpha + 2)}{2\alpha} \right] \geq 0,$$

$$w_{3,1} = \frac{1}{6} \beta_0^{\alpha-3} \alpha (\alpha - 1) \beta_1 \left[ (\alpha - 2) \beta_1^2 + 6 \beta_0 \beta_2 \right] \geq 0$$

We show that $w_m \geq 0$ for all $m \geq 4$ inductively.

$$w_{4,1} = \frac{1}{4!} \beta_0^{\alpha-4} \alpha (\alpha - 1) \left[ (\alpha - 2)(\alpha - 3) \beta_1^4 + 12(\alpha - 2) \beta_0 \beta_1^2 \beta_2 + 12 \beta_0^2 \beta_2^2 \right] \geq 0$$

$$w_{5,1} = \frac{\alpha (\alpha - 1)(\alpha - 2) \beta_0^{\alpha-5} \beta_1}{5!} \left[ (\alpha - 3)(\alpha - 4) \beta_1^4 + 20 \beta_0 \beta_1^2 \beta_2 + 60 \beta_0^2 \beta_2^2 \right] \geq 0$$

Assuming inductively that $w_{k,1}$ are non negative for $3 \leq k \leq m - 1$, we have for $m \geq 6$,

$$w_{m,1} = \frac{1}{m! \beta_0^m} \left[ (\alpha + 1 - m) w_{m-1,1,1} \beta_1 + (2\alpha + 2 - m) w_{m-2,1,2} \beta_2 \right] \geq 0 \quad \text{for} \quad 1 \leq \alpha \leq 2,$$

since $w_{m-1,1}, w_{m-2,1}, (\alpha + 1 - m), (2\alpha + 2 - m), \beta_1$ and $\beta_2$ are all non-positive for $m \geq 6$. From Corollary 1, we have the consistency condition $\sum_{k=0}^{\infty} w_k = 0$ in general which is true for $W_{2,1}(z)$ as well. Since $\sum_{k=m}^{\infty} w_{k,1} \geq 0$ for $m \geq 3$, the last inequality follows from the consistency condition. 

\[\square\]
Lemma 4. The approximation operator $\Delta_2$ is negative definite.

Proof. For any $v \in V_h$, since the diffusion coefficients $K_1, K_2$ are non-negative, we have

$$(\Delta_2 v, v) = K_1(\Delta_{2,1}^n v, v) + K_2(\Delta_{2,1}^n v, v) \leq 0.$$  \hfill \square

Theorem 3. Let $v^m = [v^m_1, v^m_2, \ldots, v^m_{N-1}]$ be the solution of the problem

$$P_h \delta_t v_i^{m+1/2} - \Delta_2 v_i^{m+1/2} = S_i^m, \quad 1 \leq i \leq N - 1, \quad 0 \leq m \leq M - 1, \quad (28)$$

$$v_0^m = 0, \quad v_M^m = 0,$$

$$v_i^0 = v_0(x_i), \quad 0 \leq i \leq N.$$

Then,

$$\|v^m\| \leq \sqrt{5} \left( \|v^0\| + \sqrt{5} \tau \sum_{l=0}^{m-1} \|S^l\| \right),$$

where $S^m = [S^m_1, S^m_2, \ldots, S^m_{N-1}]$.

Proof. Taking inner product of (28) with $v^{m+1/2}$, we have

$$(P_h \delta_t v_i^{m+1/2}, v^{m+1/2}) - (\Delta_2 v_i^{m+1/2}, v^{m+1/2}) = (S_i^m, v^{m+1/2}).$$

Since $-(\Delta_2 v_i^{m+1/2}, v^{m+1/2}) \geq 0$ from Lemma 4, we have

$$(P_h \delta_t v_i^{m+1/2}, v^{m+1/2}) \leq (S_i^m, v^{m+1/2}) = (S_i^m, v^{m+1/2})$$

$$\leq \|S^m\| \|v^{m+1/2}\| \leq \sqrt{5} \|S^m\| \|v^{m+1/2}\| P$$

$$\leq \frac{\sqrt{5}}{2} \|S^m\| \left( \|v^{m+1}\| P + \|v^m\| P \right).$$

(29)

Since $\delta_t v_i^{m+1/2} = \frac{1}{\tau}(v_i^{m+1} - v^m)$ and $v^{m+1/2} = \frac{1}{2}(v^{m+1} + v^m)$, we have

$$(P_h \delta_t v_i^{m+1/2}, v^{m+1/2}) = \left( P_h \frac{1}{\tau}(v^{m+1} - v^m), \frac{1}{2}(v^{m+1} + v^m) \right)$$

$$= \frac{1}{2\tau} \left( (P_h v^{m+1}, v^m) - (P_h v^m, v^m) \right)$$

$$= \frac{1}{2\tau} (\|v^{m+1}\|^2 P - \|v^m\|^2 P)$$

(30)

Combining (29) and (30), we have

$$\|v^{m+1}\| P \leq \|v^m\| P + \sqrt{5} \tau \|S^m\|, \quad 0 \leq m \leq M - 1.$$...
Remark 1. In the above lemma, if $P_h$ is the unit operator $I$, for the case of the order 2 with CN type scheme, since the fractional approximation operator $\Delta^{\alpha}_{h}$ is the same, the above estimate reduces to

$$
\|v^m\| \leq \|v^0\| + \tau \sum_{l=0}^{m-1} \|S^l\|, \quad 0 \leq m \leq M - 1.
$$

From the above estimates, we have the following stability result.

**Theorem 4.** The CN type difference schemes (5) of orders 2 and 3 are unconditionally stable for $1 \leq \alpha \leq 2$.

For the convergence of the approximate solution from the CN type schemes, we have the following.

**Theorem 5.** The approximate solutions of the CN type scheme (5) with the given initial and boundary conditions are convergent as $h, \tau \to 0$ for $1 \leq \alpha \leq 2$.

**Proof.** Let $e^m = u^m - \hat{U}^m$ be the error vector of the solutions, where $u^m, \hat{U}^m$ are the exact and approximate solutions of the diffusion problem (24). Then the error of the internal grid values $\hat{e}^m$ satisfy the system

$$
P_h \delta t e^{m+1/2}_i - \Delta^2 e^{m+1/2}_i = R^m_i, \quad 1 \leq i \leq N - 1, \quad 0 \leq m \leq M - 1
$$

$$
e^m_0 = 0, \quad e^m_M = 0
$$

$$
e^0_0 = 0, \quad 0 \leq i \leq N.
$$

Theorem 3 gives the estimate

$$
\|e^m\| \leq 5 \tau \sum_{l=0}^{m-1} \|R^l\| \leq 5c\tau N (\tau^2 + h^p), \quad p = 2, 3.
$$

The convergence is then established as $h, \tau \to 0$.

## 7 Numerical Results

We consider the following test example for the fractional diffusion problem (24). Let $G(x, m, \alpha) = \frac{\Gamma(m+1)}{\Gamma(a+1-\alpha)}(x^{m-a} + (1 - x)^{m-a})$ and $s_0(x) = x^5(1-x)^5$.

**Diffusion coefficients:** $K_1 = 1, K_2 = 1$,

**Source function:** $f(x, t) = -e^{-t}(s_0(x) + G(x, 5, \alpha) - 5G(x, 6, \alpha), \quad + 10G(x, 7, \alpha) - 10G(x, 8, \alpha) + 5G(x, 9, \alpha) - G(x, 10, \alpha))$,

**Initial condition:** $u(x, 0) = s_0(x)$,

**Boundary conditions:** $u(0, t) = 0, \quad u(1, t) = 0$,

**Exact Solution:** $u(x, t) = s_0(x)e^{-t}$,

**Space domain:** $0 \leq x \leq 1$,

**Time domain:** $0 \leq t \leq 1$,

The test problem was applied to the CN type numerical schemes developed in Section [24].
The second order approximation $W_{2,1}(z)$ was tested for $\alpha = 1.1, 1.5$ and 1.9. Table 5 lists the maximum error and the order of convergence for grid sizes $N = M = 16, 32, \cdots, 512$. The partition subinterval sizes are then $\tau = 1/M$ and $h = 1/N$ for time and space, respectively.

For the order 3 approximation, we choose $\tau = h^{3/2}$ to numerically realize the order 3 of the approximation operator. This means that for a space partition size $N$, we choose the time partition size $M \approx N^{3/2}$. In Table 6, the test results with the space and time partition sizes $N$ and $M$ chosen are displayed.

| $N$ | $M$ | $\|u^n - U^n\|_\infty$ | Order | $\|u^n - U^n\|_\infty$ | Order | $\|u^n - U^n\|_\infty$ | Order |
|-----|-----|-----------------|-------|-----------------|-------|-----------------|-------|
| 16  | 65  | 1.9461e-06      | 2.99  | 7.2807e-07      | 2.99  | 2.9010e-08      | 3.40  |
| 32  | 182 | 2.4807e-07      | 2.97  | 9.1351e-08      | 2.99  | 2.7484e-09      | 3.00  |
| 64  | 513 | 3.1332e-08      | 2.99  | 1.1401e-08      | 3.00  | 5.3796e-10      | 2.35  |
| 128 | 1449| 3.9404e-09      | 2.99  | 1.4224e-09      | 3.00  | 7.9399e-11      | 2.76  |
| 256 | 4097| 4.9422e-10      | 3.00  | 1.7758e-10      | 3.00  | 1.0667e-11      | 2.90  |
| 512 | 11586| 6.1888e-11     | 3.00  | 2.2183e-11      | 3.00  | 1.3792e-12      | 2.95  |

Table 6: Order 3 convergence of CN type scheme

These test results show that the second order approximation and the third order approximation operator with $W_{2,1}$ are justified for their order of convergence and unconditional stability with the CN type schemes.

## 8 Conclusion

A generalization of the Grünwald approximation for the left and right fractional derivatives are presented in terms of generating functions. Using this generalization, a second order difference approximation is constructed. A quasi-compact approximation of order 3 is also obtained by using the second order approximation operators with a preconditioner operator. The approximations are first tested for steady state problems and numerically confirmed their theoretical order. Numerical schemes for these approximations to solve fractional diffusion equations are devised with proof of stability and convergence. The theoretical developments are tested and verified for time dependent diffusion problems through an example. The approach of generating functions might be a useful tool for constructing difference approximation formulas for fractional derivatives.

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