A tunable finite difference method for fractional differential equations with non-smooth solutions

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Highlights

- A FDM of tunable accuracy for FDEs with end-point singularities is developed.
- WSGL formulas with correction terms are proposed to discretize fractional derivatives.
- Satisfactory numerical solutions can be obtained by tuning the correction terms.
- Numerical examples verify the effectiveness of the present method.

Abstract

In this work, a finite difference method of tunable accuracy for fractional differential equations (FDEs) with end-point singularities is developed. Modified weighted shifted Gr"{u}nwald–Letnikov (WSGL) formulas are proposed to approximate the left and right Riemann–Liouville fractional operators, which show better accuracy than the original WSGL formulas, due to the use of the correction terms. Finite difference schemes are constructed to solve two fractional boundary value problems and a space-fractional Allen–Cahn equation. Even if the singularity of the considered FDEs is unknown, satisfactory numerical solutions can still be obtained by suitably tuning the correction terms. Various numerical examples are presented to verify the effectiveness of the present method, and comparisons with other known methods are also made that demonstrate higher accuracy of the current method.

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1. Introduction

This paper aims to provide a numerical method with tunable accuracy to solve the FDEs with end-point singularities. Because the fractional operators are nonlocal with weakly singular kernels, the fractional models are more complicated than the classical models. Hence, the solutions of fractional models are also more complicated and they are often non-smooth. There are several analytical methods to solve fractional differential equations, such as the
Table 1
Number of positive eigenvalues of the matrix $L_{A^{(α,m)}_{1,0}}$ defined in (16), $σ_k = 0.1k$, and $N = 128$.

<table>
<thead>
<tr>
<th>$α$</th>
<th>$m = 0$</th>
<th>$m = 1$</th>
<th>$m = 2$</th>
<th>$m = 3$</th>
<th>$m = 4$</th>
<th>$m = 5$</th>
<th>$m = 6$</th>
</tr>
</thead>
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<tr>
<td>1.05</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1.1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1.2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1.3</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
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<tr>
<td>1.4</td>
<td>0</td>
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<td>0</td>
<td>0</td>
<td>0</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>1.5</td>
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<td>0</td>
<td>0</td>
<td>0</td>
<td>2</td>
<td>2</td>
</tr>
</tbody>
</table>

Fourier transform method, the Laplace transform method, the Mellin transform method, the Green’s function method, and so on [1–5]. However, analytical methods do not work well on most of FDEs, e.g. with non-constant coefficients or non-linearities. Hence, developing numerical methods is of great importance in practical applications.

There have been various numerical methods to solve FDEs, such as finite difference methods [6–13], finite element methods [14–19], and spectral methods [20–26]. However, most of the known methods work well on FDEs with smooth solutions (or solutions with relatively good regularities). Unlike the classical differential equations, solutions to FDEs are generally non-smooth. For example, given smooth initial/boundary conditions and source terms, the solutions of FDEs are non-smooth and even have stronger singularity at the boundaries, which have not been properly resolved in recent works, see e.g. [1,5,25,27,28]. Up to now, a few numerical methods have been proposed for FDEs with non-smooth solutions, such as the use of non-uniform grids (see e.g. [29–33]), the non-polynomial/singular basis (see e.g. [21,28,34,25–27,35]), and Lubich’s correction method (see e.g. [36–40]). Lubich’s method consists of adding suitable correction terms to the corresponding numerical approximation, which makes the new approximation exact for low regularity terms of the solutions while still maintaining high accuracy for high regularity terms.

In this work, we extend Lubich’s correction method to solve fractional boundary value problems with end-point singularities. Specifically, we add correction terms to the weighted shifted Grünwald–Letnikov (WSGL) formulas proposed in [41], which were proved to lead to second-order accuracy under some restrictive conditions. Here, we prove that the left (or right) WSGL formula is a second-order approximation of the left (or right) Riemann–Liouville (RL) fractional operator far from the origin under weaker conditions, see Lemma 2.1 and numerical verifications in Example 2.1. Following Lubich’s method, we first add correction terms to the left WSGL formula to obtain the modified left WSGL formula that can keep global second-order accuracy. The accuracy of the modified WSGL formula depends on two factors: the number of the correction terms and the residue of the ill-conditioned linear system to derive the starting weights used in the correction terms [42,36]. Thanks to the small factor in the error equation induced by the correction terms (see $S_{σ_m}$ in Lemma 2.2 and related results in [40]), we do not need many correction terms to get high accurate numerical solutions. Therefore, we avoid solving the ill-conditioned linear system with large condition number, which makes our method more practical in real applications. Numerical tests in Examples 2.2 and 4.1 demonstrate that just a few correction terms are enough to obtain high accurate numerical solutions.

We also studied how to add correction terms such that the modified WSGL formula achieves high accuracy when the solution to the considered FDE has singularities at both end-points. One important feature is that the correction indices (see $\{σ_r\}$ used in (7)) can be flexible and do not need to be the exact singularity indices of the analytical solution, and hence high accuracy of the modified WSGL formula can still be obtained; this aspect was not investigated in the pioneering work by Lubich [36], see theoretical explanation in Lemma 2.2.

We explore numerically the eigenvalues of the matrix derived from the modified WSGL formula, and find that the eigenvalues are influenced by the fractional orders, the correction indices (see $\{σ_r\}$ used in (7)), and the number of the correction terms ($m$ in (7)), see numerical results in Tables 1–3. Numerical simulations demonstrate that even two correction terms are sufficient to obtain satisfactory numerical solutions. Comparisons with the known methods are also made to illustrate the good performance of the present method.

This paper is organized as follows. In Section 2, we derive the second-order accurate modified WSGL formula by adding correction terms to the original WSGL formula, which is applied to solve the fractional boundary value problems with one-sided fractional derivative. In Section 3, we extend the modified WSGL formula to discretize the left and right Riemann–Liouville (RL) fractional derivatives. The tunable finite difference method is constructed to
solve the fractional boundary value problems with two-sided fractional derivatives. In Section 4, some numerical experiments are given to illustrate the effectiveness of our algorithms before we present the conclusion in Section 5.

2. Fractional boundary value problems with one-sided fractional derivative

In this section, we focus on the discretization of the left fractional derivative operator. By examining the error equation of the original WSGL formula and following Lubich’s approach [36], we introduce proper correction terms to the original WSGL formula to obtain a new discretization. Then the finite difference scheme is constructed to solve the following fractional boundary value problem [43],

\[
\begin{cases}
-\mathcal{D}_L^{\alpha} U(x) + b(x) \mathcal{D}^{\alpha-1} U(x) + c(x) U(x) = f(x), & x \in (x_L, x_R), \\
U(x_L) = 0, & U(x_R) = 0,
\end{cases}
\]

where $1 < \alpha \leq 2$, $b(x), c(x) \geq 0$, and $\mathcal{D}_L^{\alpha}$ is the left RL fractional derivative operator defined by

\[
\mathcal{D}_L^{\alpha} U(x) = \frac{1}{\Gamma(2-\alpha)} \frac{d^2}{dx^2} \int_{x_L}^x (x - s)^{1-\alpha} U(s) \, ds.
\]

The right RL fractional derivative operator $\mathcal{D}_R^{\alpha}$ is also used in this paper, which is defined by

\[
\mathcal{D}_R^{\alpha} U(x) = \frac{1}{\Gamma(2-\alpha)} \frac{d^2}{dx^2} \int_x^{x_R} (s - x)^{1-\alpha} U(s) \, ds.
\]
The proof of this lemma is similar to Eq. (2.7) in [40], and hence it is omitted here.

Proof. Let \( h \) be the stepsize and \( N \) be a positive integer with \( h = (x_R - x_L)/N \). The grid point \( x_i \) is given as \( x_i = x_L + i h \) (i = 0, 1, ..., N).

The modified WSGL formula will be employed to discretize the fractional derivative in Eq. (1). We first present the WSGL proposed in [41], which is given by

\[
L A_{h,p,q}^{\alpha,i} U = \frac{\alpha - 2q}{2(p-q)} L A_{h,p}^{\alpha,i} U + \frac{2p - \alpha}{2(p-q)} L A_{h,q}^{\alpha,i} U, \quad p, q \in \mathbb{Z},
\]

(4)

where \( A_{h,p}^{\alpha,i} \) is the shifted Grünwald–Letnikov formula with \( p \) shifts, which is given by

\[
L A_{h,p}^{\alpha,i} U = \frac{1}{h^\alpha} \sum_{k=0}^{i+p} \omega_k(\alpha) U(x_{i-k+p}) = \frac{1}{h^\alpha} \sum_{k=0}^{i+p} \omega_k(\alpha) U_{i-k+p}, \quad \omega_k(\alpha) = (-1)^k \binom{\alpha}{k}.
\]

(5)

In [41], the approximation \( L A_{h,p,q}^{\alpha,i} U \) is proved to be of second-order convergence when \( U(x_L) = 0 \), \( RL D_{xL,x}^{\alpha+2} U(x) \) and its Fourier transform belong to \( L_1(\mathbb{R}) \). Obviously, these conditions are too restrictive since \( RL D_{xL,x}^{\alpha+2} U(x) \not\in L_1(\mathbb{R}) \) even for smooth \( U(x) = x - x_L \). In fact, \( L A_{h,p,q}^{\alpha,i} U \) is a second-order approximation of \( RL D_{xL,x}^{\alpha+2} U(x)|_{x=x_i} \) if \( x_i \) is far from the origin \( x = x_L \), when \( U(x) = (x - x_L)^\sigma, \sigma > 0 \), see the following lemma.

Lemma 2.1. Let \( U(x) = (x - x_L)^\sigma, \sigma \geq 0 \) and \( p, q \in \mathbb{Z} \). Then

\[
\left| RL D_{xL,x}^{\alpha} U(x)|_{x=x_i} - L A_{h,p,q}^{\alpha,i} U \right| \leq C h^\sigma |\alpha|^{\sigma - |\alpha| - 2} = C h^2 (x_i - x_L)^{\sigma - |\alpha| - 2}.
\]

(6)

Proof. The proof of this lemma is similar to Eq. (2.7) in [40], and hence it is omitted here.

Example 2.1. Let \( U(x) = x + x^2 + x^3 + x^4, x \in (0, 1) \). Use the WSGL formula (4) with \( (p, q) = (1, 0) \) (see also (9)) to numerically calculate \( RL D_{0,x}^{\alpha} U(x) \).

Let \( \xi_i = RL D_{0,x}^{\alpha} U(x)|_{x=x_i} - L A_{h,1.0}^{\alpha,i} U \). Then we display the pointwise errors \( |\xi_i| \) in Fig. 2.1(a) for \( \alpha = 1.5 \). We can see that second-order accuracy is observed when \( i \) is sufficiently large (see Lemma 2.1), i.e., \( x_i \) is far from the origin \( x = 0 \). However, large error occurs near the origin \( x = 0 \). The convergence rate of \( L A_{h,1.0}^{\alpha,i} U \) is \( O(h^{1-\alpha}) \) near \( x = 0 \) in this example, since the term \( x \) in \( U(x) \) determines the convergence rate, and this error is not improved significantly even if the small step size \( h = N^{-1} \) is employed, see Fig. 2.1(a). Fig. 2.1(b) shows the \( L^2 \) error \( \sqrt{h \sum_{i=1}^{N} \xi_i^2} \) of the discrete operator \( L A_{h,1.0}^{\alpha,i} \) for \( \alpha = 1.1, 1.5, 1.9 \). From (6), we can easily obtain \( \sqrt{h \sum_{i=1}^{N} \xi_i^2} \leq C h^{1.5-\alpha} \) in this example, which is also verified in Fig. 2.1(b).
Fig. 2.1 demonstrates that the WSGL formula (4) is not a good approximation of $RL D^{\alpha, i, m}_{x_L, x}$ even if $U(x)$ is smooth in (4), which can also be explained from Lemma 2.1. In order to remedy the accuracy loss of the WSGL formula, we employ Lubich’s approach [36] by introducing correction terms into (4) to get the modified WSGL formula, which preserves higher accuracy compared to the original WSGL formula. The modified WSGL formula is given by

$$L A^{\alpha, i, m}_{h, p, q} U = L A^{\alpha, i, m}_{h, p, q} U + \frac{1}{h^{\alpha}} \sum_{k=1}^{m} q_{i,k}^{(\alpha)} U_k,$$

where $\{q_{i,k}^{(\alpha)}\}$ are called the starting weights that are chosen in order that (7) is exact for some $U(x) = (x - x_L)^{\sigma}$, $\sigma > 0$, $1 \leq r \leq m$, i.e., $RL D^{\alpha, i, m}_{x_L, x} U(x)|_{x = x_L} = L A^{\alpha, i, m}_{h, p, q} U$ for $U(x) = (x - x_L)^{\sigma}$. Here $\sigma$ is also called the correction index. As in [41], we can choose $(p, q) = (1, 0)$ or $(p, q) = (1, -1)$ in the numerical tests and simulations in this paper. Specifically, the starting weights $\{q_{i,k}^{(\alpha)}\}$ can be solved from the following linear system

$$\sum_{k=1}^{m} q_{i,k}^{(\alpha)} k^{\sigma r} = \frac{\Gamma(\sigma r + 1)}{\Gamma(\sigma r + 1 - \alpha)} r^{\sigma r - \alpha} - \sum_{k=0}^{i+1} g_{i+1-k}^{(\alpha)} k^{\sigma r}, \quad 1 \leq r \leq m,$$

where $g_{k}^{(\alpha)}$ satisfies:

- For $(p, q) = (1, 0)$, the coefficient $g_{k}^{(\alpha)}$ is given by

$$g_{0}^{(\alpha)} = \frac{\alpha}{2} \omega_{0}^{(\alpha)}, \quad g_{k}^{(\alpha)} = \frac{\alpha}{2} \omega_{k}^{(\alpha)} + \frac{2 - \alpha}{2} \omega_{k-1}^{(\alpha)}, \quad k \geq 1.$$

If $\alpha \to 1$, then (9) is reduced to $g_{0}^{(1)} = 1/2, g_{1}^{(1)} = 0, g_{2}^{(1)} = -1/2$ and $g_{k}^{(1)} = 0$ for $k \geq 3$.

- For $(p, q) = (1, -1)$, the coefficient $g_{k}^{(\alpha)}$ is given by

$$g_{0}^{(\alpha)} = \frac{2 + \alpha}{4} \omega_{0}^{(\alpha)}, \quad g_{1}^{(\alpha)} = \frac{2 + \alpha}{4} \omega_{1}^{(\alpha)}, \quad g_{k}^{(\alpha)} = \frac{2 + \alpha}{4} \omega_{k}^{(\alpha)} + \frac{2 - \alpha}{4} \omega_{k-2}^{(\alpha)}, \quad k \geq 2.$$

If $\alpha \to 1$, then (10) is reduced to $g_{0}^{(1)} = 3/4, g_{1}^{(1)} = -3/4, g_{2}^{(1)} = 1/4, g_{3}^{(1)} = -1/4$ and $g_{k}^{(1)} = 0$ for $k \geq 4$.

**Remark 2.1.** As pointed out in [42,36], the linear system (8) is ill-conditioned when $m$ is sufficiently large. However, we only need just a few correction terms to get satisfactory accuracy in real applications, which yields a modest condition number when $m$ in (8) is not too big; see detailed discussion in [40].

The following lemma gives an error bound for the modified WSGL formula (7).

**Lemma 2.2.** Let $U(x) = (x - x_L)^{\sigma}, \sigma > 0, p, q \in \mathbb{Z}, p \neq q, \text{ and } m \in \mathbb{Z}^+$. Then there exists two positive constants $C$ and $\tilde{C}$ independent of $i$ and $h$ such that

$$|RL D^{\alpha}_{x_L, x} U(x)|_{x=x_L} - L A^{\alpha, i, m}_{h, p, q} U| \leq h^{\sigma - \alpha} \left[ C S^{\sigma}_{m} \left( i^{\sigma - \alpha} \log^{m}(i) + d_{0} \right) + \tilde{C} i^{\sigma - \alpha} \right],$$

where $\sigma_{\max} = \max(\sigma_1, \sigma_2, \ldots, \sigma_m, \sigma), S^{\sigma}_{m} = \prod_{k=1}^{m} |\sigma - \sigma_k|$, and $d_{0}$ is a suitable positive integer.

**Proof.** The proof is similar to Lemma 2.2 in [40], and hence it is omitted here. □

Numerical simulations reveal a better upper bound of $|RL D^{\alpha}_{x_L, x} U(x)|_{x=x_L} - L A^{\alpha, i, m}_{h, p, q} U|$, which is given below:

$$|RL D^{\alpha}_{x_L, x} U(x)|_{x=x_L} - L A^{\alpha, i, m}_{h, p, q} U| \leq C S^{\sigma}_{m} h^{\sigma - \alpha} i^{\sigma_{\max} - \alpha - 2}.$$

Readers can refer to [40] for more discussion and numerical results.

**Example 2.2.** Let $U(x) = x + x^2 + x^3 + x^4, x \in (0, 1)$. Use the modified WSGL formula (7) with different number of correction terms to approximate $RL D^{\alpha}_{0, x} U(x)$. 

The aim of Example 2.2 is to demonstrate that the correction terms in $L^{A_{h,p,q}}_{\alpha \in \mathbb{R}^+}$ can significantly improve the accuracy of the original WSGL formula $L^{A_{h,p,q}}_{\alpha = 1}$, even if the correction indices $\{\hat{\sigma}_k\}$ in $L^{A_{h,p,q}}_{\alpha \in \mathbb{R}^+}$ do not match exactly the regularity indices $\{\sigma_k\}$ of the analytical solution $U(x) = \sum_{k=1}^{\infty} c_k (x - x_L)^{\hat{\sigma}_k} (0 < \hat{\sigma}_k < \hat{\sigma}_{k+1})$. If $\{\sigma_1, \ldots, \sigma_m\} = \{\hat{\sigma}_1, \ldots, \hat{\sigma}_m\}$, then best numerical approximations will be achieved, see Fig. 2.2(a), where we observe significant improvement of accuracy as the number of correction terms $m$ increases. However, we may not know the regularity index $\hat{\sigma}_k$ of the analytical solution $U(x)$ to the considered FDEs. In such a case, we can still obtain good accuracy improvement of the discrete operator $L^{A_{h,p,q}}_{\alpha \in \mathbb{R}^+}$ as long as $S^{\hat{\sigma}_k} \big|_{\hat{\sigma}_k = 1} = \min_{1 \leq k \leq m} |\sigma_k - \hat{\sigma}_1|$ is sufficiently small; see numerical results in Fig. 2.2(b), where we have $\hat{\sigma}_1 = 1$ in this example and the term $x^{\hat{\sigma}_1} (\hat{\sigma}_1 = 1)$ dominates the convergence of $L^{A_{h,p,q}}_{\alpha \in \mathbb{R}^+}$ when $\hat{\sigma}_1 \notin \{\sigma_1, \ldots, \sigma_m\}$. Numerical tests show that the smaller value of $S^{\hat{\sigma}_k} \big|_{\hat{\sigma}_k = 1}$, the better accuracy of $L^{A_{h,p,q}}_{\alpha \in \mathbb{R}^+}$, we refer readers to [40] for more details and explanations. This positive effect of $S^{\hat{\sigma}_k} \big|_{\hat{\sigma}_k = 1}$ on the improvement of accuracy of $L^{A_{h,p,q}}_{\alpha \in \mathbb{R}^+}$ will also be verified in the numerical simulations in Section 5.

We also present the $L^2$ errors of $L^{A_{h,p,q}}_{\alpha \in \mathbb{R}^+}$ in Fig. 2.2(c) and (d). We can see that second-order accuracy is observed in Fig. 2.2(c) as the number of correction terms increases due to the fact that $\sigma_k$ in $L^{A_{h,p,q}}_{\alpha \in \mathbb{R}^+}$ matches the regularity index of $U(x)$. We do not observe second-order accuracy as the number of correction terms increases in Fig. 2.2(d), since $\sigma_k$ in $L^{A_{h,p,q}}_{\alpha \in \mathbb{R}^+}$ does not exactly match the regularity index of $U(x)$. However, the accuracy is improved, which can be explained from the smaller coefficient $S^\sigma_m$ in the error bound in Lemma 2.2 (see also (12)). Here $\sigma = 1$ and $S^1_m = 10^{-m}m!$ in Fig. 2.2(d) and the term $x$ in $U(x)$ dominates the convergence rate and accuracy.
Letting \( x = x_i \) (1 \( \leq i \leq N - 1 \)) in (1), we have
\[
-L \mathcal{A}^{\alpha, i, 0} U + b_i L \mathcal{A}^{\alpha, 0, i} U + c_i U_i = f_i + R_i,
\]
where \( L \mathcal{A}^{\alpha, i, 0} \) is defined by (7) and \( R_i \) is the truncation error. If the analytical solution \( U(x) \) satisfies \( U(x) = \sum_{k=1}^{\infty} c_k (x - x_L)^k \), then from (12), the truncation error \( R_i \) satisfies
\[
|R_i| \leq C h^2 (x_i - x_L)^{\sigma_n + 1 - \alpha - 2}.
\]

Let \( u_i \) be the approximate solution of \( U(x_i) \). Then, from (13), we derive the fully discrete FDM for (1) as: Find \( u_i \) for \( i = 1, 2, \ldots, N - 1 \) such that
\[
-L \mathcal{A}^{\alpha, i, 0} U + b_i L \mathcal{A}^{\alpha, 0, i} U + c_i U_i = f_i,
\]
where \( L \mathcal{A}^{\alpha, i, 0} \) is defined by (7) and \((p, q) = (1, 0)\) or \((0, 1)\).

Let \( \left( L \mathcal{A}^{\alpha, 1, 0} U, L \mathcal{A}^{\alpha, 2, 0} U, \ldots, L \mathcal{A}^{\alpha, N-1, 0} U \right)^T = \frac{1}{h^\alpha} L \mathcal{A}^{(\alpha, m)} u \), where \( u = (u_1, u_2, \ldots, u_{N-1})^T \). Then the matrix representation of the method (15) is given by
\[
\left( -\frac{1}{h^\alpha} L \mathcal{A}^{(\alpha, m)} + \frac{1}{h} \text{diag}(b) L \mathcal{A}^{(1, m)} + \text{diag}(c) \right) u = f,
\]
where \( b = (b_1, b_2, \ldots, b_{N-1})^T \) and \( c = (c_1, c_2, \ldots, c_{N-1})^T \). For \( 1 < \alpha \leq 2 \) and \( m = 0 \), the matrix \( L \mathcal{A}^{(\alpha, 0)} \) is negative definite [41], but this may not be true when \( m > 0 \) is sufficiently large. Fortunately, numerical simulation shows that the eigenvalues of \( L \mathcal{A}^{(\alpha, m)} \) have negative real part when \( m \) is not too large and the fractional order \( \alpha \) is small, for example, \( \alpha = 1.1 \). Table 1 displays the number of eigenvalues with positive real parts of the matrix \( L \mathcal{A}^{(\alpha, m)} \) defined in (16). We can see that all the real parts of the eigenvalues of \( L \mathcal{A}^{(\alpha, m)} \) are negative for \( m \leq 6 \) and \( \alpha = 1, 1.1, 1.2, 1.3 \), while for \( \alpha = 1.4, 1.5 \), the eigenvalues of the matrix \( L \mathcal{A}^{(\alpha, m)} \) have negative real parts when \( m \leq 3 \) and \( \alpha \leq 1.3 \). If we set \( \sigma = 1 + 0.1 k \) in the computation, then we find that all the eigenvalues of the matrix \( L \mathcal{A}^{(\alpha, m)} \) have negative real parts for \( m \leq 6 \) and \( \alpha \leq 1.7 \).

3. Fractional boundary value problems with two-sided fractional derivatives

This section focuses on the following fractional boundary value problem with two-sided fractional derivatives [27],
\[
\begin{align*}
- \left( \epsilon_1(x) L \mathcal{D}_{x}^{\alpha, 0} U(x) + \epsilon_2(x) R \mathcal{D}_{x}^{\alpha, 0} U(x) \right) & U(x) + c(x) U(x) = f(x), & x \in (x_L, x_R), \\
U(x_L) & = U(x_R) = 0,
\end{align*}
\]
where \( 1 < \alpha_1, \alpha_2 \leq 2 \), \( L \mathcal{D}_{x}^{\alpha, 0} \) and \( R \mathcal{D}_{x}^{\alpha, 0} \) are the left and right RL fractional operators, respectively. The diffusion coefficients \( \epsilon_k \) (\( k = 1, 2 \)) satisfy \( \epsilon_k \geq 0 \) and \( \epsilon_1^2 + \epsilon_2^2 \neq 0 \).

In Section 2, we introduced the (modified) WSGL formula for the left RL fractional operator appeared in the FBVPs (1). Here, we extend the modified WSGL formula in the previous section to discretize both the left and right RL fractional derivative operators in (17).

Next, we introduce two ways to add the correction terms to the left WSGL formula, which are given by
\[
\begin{align*}
L \mathcal{D}_{x}^{\alpha, i, 0} U & = L \mathcal{A}_{h, p, q}^{\alpha, i} U + \frac{1}{h^\alpha} \sum_{k=1}^{m} \phi_{i,k}^{(\alpha)} U_k, \\
R \mathcal{D}_{x}^{\alpha, i, 0} U & = L \mathcal{A}_{h, p, q}^{\alpha, i} U + \frac{1}{h^\alpha} \sum_{k=1}^{m} \phi_{i,k}^{(\alpha)} U_{N-k},
\end{align*}
\]
where \( \phi_{i,k}^{(\alpha)} \) in (18) are chosen in order that \[ L \mathcal{D}_{x}^{\alpha, i, 0} U(x)=\frac{1}{x_{i}^{\alpha}} R \mathcal{D}_{x}^{\alpha, i, 0} U \] for \( U(x) = (x - x_L)^{\sigma_r} (x_R - x)^{\delta_r}, \sigma_r, \delta_r \geq 0, 1 \leq r \leq m \), and \( \phi_{i,k}^{(\alpha)} \) in (19) satisfy \[ L \mathcal{D}_{x}^{\alpha, i, 0} U(x)=\frac{1}{x_{i}^{\alpha}} L \mathcal{D}_{x}^{\alpha, i, 0} U \] for \( U(x) = (x - x_L)^{\sigma_r} (x_R - x)^{\delta_r} \).
x) = \hat{x}_r, \hat{\sigma}_r, \hat{\delta}_r \geq 0, 1 \leq r \leq m. Specifically, for (p, q) = (1, 0) or (1, -1) (see (9) or (10)), the starting weights \( \{ \varphi_{i,k}^{(\alpha)} \} \) in (18) can be obtained from the following linear system

\[
\sum_{k=1}^{m} \varphi_{i,k}^{(\alpha)} (1 + \hat{x}_k)^{\sigma_r} (1 - \hat{x}_k)^{\hat{\delta}_r} = \frac{2^{\hat{\delta}_r} (1 + \hat{x}_k)^{\hat{\sigma}_r - \alpha} \Gamma(\sigma_r + 1)}{\Gamma(\hat{\sigma}_r + 1 - \alpha)} 2F_1 \left( -\delta_r, \sigma_r + 1; -\alpha + \sigma_r + 1; \frac{1 + \hat{x}_k}{2} \right) - \sum_{k=0}^{i+1} g_{i+1,k}^{(\alpha)} (1 + \hat{x}_k)^{\sigma_r} (1 - \hat{x}_k)^{\hat{\delta}_r}, \quad 1 \leq r \leq m, \tag{20}
\]

and the starting weights \( \{ \varphi_{i,k}^{(\alpha)} \} \) in (19) can be obtained from the following linear system

\[
\sum_{k=1}^{m} \varphi_{i,k}^{(\alpha)} (1 + \hat{x}_{N-k})^{\hat{\sigma}_r} (1 - \hat{x}_{N-k})^{\hat{\delta}_r} = \frac{2^{\hat{\delta}_r} (1 + \hat{x}_k)^{\hat{\sigma}_r - \alpha} \Gamma(\hat{\sigma}_r + 1)}{\Gamma(\hat{\sigma}_r + 1 - \alpha)} 2F_1 \left( -\hat{\delta}_r, \hat{\sigma}_r + 1; -\alpha + \hat{\sigma}_r + 1; \frac{1 + \hat{x}_k}{2} \right) - \sum_{k=0}^{i+1} g_{i+1,k}^{(\alpha)} (1 + \hat{x}_k)^{\hat{\sigma}_r} (1 - \hat{x}_k)^{\hat{\delta}_r}, \quad 1 \leq r \leq m, \tag{21}
\]

where \( \hat{x}_k = -1 + 2k/N \) and \( 2F_1(a, b; c; z) \) is the hypergeometric function defined by

\[
2F_1(a, b; c; z) = \sum_{k=0}^{\infty} \frac{(a)_k (b)_k}{(c)_k (k+1)} z^k = \frac{\Gamma(c)}{\Gamma(b) \Gamma(c-b)} \int_0^1 (1-s)^{c-b-1} s^{b-1} (1-zs)^{-a} ds,
\]

in which \( (a)_k = \frac{\Gamma(a+k)}{\Gamma(a)} \), \( b > 0 \). There are many numerical approaches to efficiently calculate the hypergeometric function \( 2F_1(a, b; c; z) \), see for example [44,45].

Next, we test the accuracy of \( \frac{\tilde{L}_{B_{h,1,0}^{\sigma,i,m}}}{} \) and show how the correction terms affect the accuracy of \( \frac{\tilde{L}_{B_{h,1,0}^{\sigma,i,m}}}{} \).

**Example 3.1.** Let \( U(x) = (1 + x)^{\sigma} (1 - x)^{\delta}, x \in (-1, 1), \sigma = 0.11 \) and \( \delta = 1.05 \). Use the modified WSGL formula (18) and (19) with different number of correction terms to approximate \( RL D_{-1,x}^{\sigma} U(x) \).

- **Case I:** Let \( \sigma_k = 0.1k \) and \( \delta_k = 0, \hat{\delta}_k = 1, \delta_k = 1.05, \) or \( \delta_k = 0.9 + 0.1k \) in \( \frac{\tilde{L}_{B_{h,1,0}^{\sigma,i,m}}}{} \),

- **Case II:** Let \( \hat{\sigma}_k = 0.9 + 0.1k \) and \( \hat{\delta}_k = 0, \sigma_k = 0.1, \hat{\delta}_k = 0.11, \) or \( \hat{\delta}_k = 0.1k \) in \( \frac{\tilde{L}_{B_{h,1,0}^{\sigma,i,m}}}{} \).

We choose \( U(x) = (1 + x)^{\sigma} (1 - x)^{\delta} \) since the solution to (17) may contain the singular term \( (1 + x)^{\sigma} (1 - x)^{\delta} \), and \( \sigma \) and/or \( \delta \) may be very small and hence they may dominate the accuracy of the existing numerical methods, see [46,27]. It is easy to find that there are several optimal choices of \( \sigma_k, \hat{\sigma}_k, \hat{\sigma}_k, \delta_k, m \) in \( \frac{\tilde{L}_{B_{h,1,0}^{\sigma,i,m}}}{} \) that make

\[
e_i^\pm = \frac{\tilde{L}_{B_{h,1,0}^{\sigma,i,m}}}{RL D_{-1,x}^{\sigma,i,m}} U(x) = 0. \]

For example, one optimal choice is \( m = 1, \sigma_1 = \sigma, \delta_1 = \delta \) for \( \frac{\tilde{L}_{B_{h,1,0}^{\sigma,i,m}}}{} \) and \( m = 1, \hat{\sigma_1} = \sigma, \hat{\delta}_1 = \delta \) for \( \frac{\tilde{L}_{B_{h,1,0}^{\sigma,i,m}}}{} \). Here, we do not take those optimal choices in Cases I–II, since we may not exactly know \( \sigma \) and \( \delta \) in real applications. We mainly focus on how \( \prod_{k=1}^{m} |\sigma - \sigma_k| \) (or \( \prod_{k=1}^{m} |\delta - \delta_k| \)) affects the accuracy of \( \frac{\tilde{L}_{B_{h,1,0}^{\sigma,i,m}}}{} \) (or \( \frac{\tilde{L}_{B_{h,1,0}^{\sigma,i,m}}}{} \)).

The pointwise errors \( |e_i^\pm| \) for Case I are displayed in Fig. 3.1. Compared with the original WSGL formula \( \frac{\tilde{L}_{B_{h,1,0}^{\sigma,i,m}}}{} \), the modified WSGL formula \( \frac{\tilde{L}_{B_{h,1,0}^{\sigma,i,m}}}{} (m > 0) \) with suitable correction terms achieves significant improvement of accuracy, see the absolute errors in Fig. 3.1a)–(d) near \( x = -1 \) for \( m \geq 3 \). However, we find from Fig. 3.1a), (b) and (d) that there is not obvious accuracy improvement for \( \frac{\tilde{L}_{B_{h,1,0}^{\sigma,i,m}}}{} (m > 0) \) near the right end-point \( x = 1 \) when \( \delta_k \neq \delta \). This is caused by the singularity of \( U(x) \) near the right end-point \( x = 1 \). If \( \delta \) is a nonnegative integer, then the discrete operator \( \frac{\tilde{L}_{B_{h,1,0}^{\sigma,i,m}}}{} \) is a good approximation of \( RL D_{-1,x}^{\sigma,i,m} \) far from \( x = -1 \), which is also verified in Examples 2.1 and 2.2.

Next, we will show that the discrete operator \( \frac{\tilde{L}_{B_{h,1,0}^{\sigma,i,m}}}{} (m > 0) \) is a good approximation of \( RL D_{-1,x}^{\sigma,i,m} \) near \( x = 1 \) by choosing suitable correction terms. The parameters are taken as in Case II, and the absolute errors \( |e_i^-| \) are displayed in Fig. 3.2. We can see that the discrete operator \( \frac{\tilde{L}_{B_{h,1,0}^{\sigma,i,m}}}{} (m > 0) \) with suitable correction terms really shows much better approximation than that of the original WSGL formula near \( x = 1 \).
Fig. 3.1. Pointwise errors $L^\alpha_{h,p,q}$ for Example 3.1, Case I, $\sigma_k = 0.1k$, $N = 128$, and $\alpha = 1.1$.

From Figs. 3.1 and 3.2, we observe that there exists at least a nonnegative integer $d$, such that the following discrete operator

\[
L^\alpha_{h,p,q} U = \begin{cases} 
L^\alpha_{h,p,q} U, & i \leq d, \\
- L^\alpha_{h,p,q} U, & i > d
\end{cases}
\]  

is a good approximation of $\mathcal{R}_x^\alpha$. From Figs. 3.1 and 3.2, we can choose $d = 7\lceil N/8 \rceil$ and display the absolute errors of $L^\alpha_{h,1,0} U$ in Fig. 3.3, where $\sigma_k = 0.1k, \hat{\delta}_k = 1$ in $L^\alpha_{h,p,q} U$ when $i \leq d$ and $\hat{\delta}_k = 0.1, \hat{\delta}_k = 0.9 + 0.1k$ in $L^\alpha_{h,p,q} U$ when $i > d$. We can see that the discrete operator $L^\alpha_{h,1,0} U$ combines the advantages of the discrete operators $L^\alpha_{h,1,0} U$ and $L^\alpha_{h,1,0} U$, and displays better accuracy than that of $L^\alpha_{h,1,0} U$.

Approximating to $\mathcal{R}_x^\alpha$, the discrete operator $R^\alpha_{h,p,q} U$ can be defined similarly as

\[
R^\alpha_{h,p,q} U = \begin{cases} 
R^\alpha_{h,p,q} U, & i \leq d, \\
- R^\alpha_{h,p,q} U, & i > d
\end{cases}
\]

where

\[
R^\alpha_{h,p,q} U = R^\alpha_{h,p,q} U + \frac{1}{h^\alpha} \sum_{k=1}^{m} \psi_{i,k}(a) U_{N-k},
\]

\[
- R^\alpha_{h,p,q} U = R^\alpha_{h,p,q} U + \frac{1}{h^\alpha} \sum_{k=1}^{m} \psi_{i,k}(a) U_{N-k}.
\]
Fig. 3.2. Pointwise errors of $L^R\alpha, i, m, h, 1, 0$ for Example 3.1, Case II, $\delta_k = 0.9 + 0.1k$, $N = 128$, and $\alpha = 1.1$.  

In which $R^A_{h,p,q}$ is the WSGL formula for the right RL fractional operator (see [41]) defined by

$$R^A_{h,p,q} U = \frac{\alpha - 2q}{2(p - q)} R^A_{h,p} U + \frac{2p - \alpha}{2(p - q)} R^A_{h,q} U, \quad p, q \in \mathbb{Z}. \quad (26)$$

Here, $R^A_{h,p}$ is the right shifted Grünwald–Letnikov formula (with $p$ shifts) defined by

$$R^A_{h,p} U = \frac{1}{h^\alpha} \sum_{k=0}^{N-i+p} \omega_k^{(\alpha)} U_{i+k-p}, \quad \omega_k^{(\alpha)} = (-1)^k \binom{\alpha}{k}. \quad (27)$$

The starting weights $\{\psi_k^{(\alpha)}\}$ in (24) (or (25)) are chosen such that $R^B_{h,p,q} U = [RLD_{x\in x_L} U(x)]_{x=x_i}$ (or $R^B_{h,p,q} U = [RLD_{x\in x_R} U(x)]_{x=x_i}$) for $U(x) = (x - x_L)^{\hat{\sigma}_k} (x_R - x)^{\hat{\delta}_k}$ (or $U(x) = (x - x_L)^{\hat{\sigma}_k} (x_R - x)^{\hat{\delta}_k}$). Specifically, the starting weights $\{\psi_k^{(\alpha)}\}$ in (24) (or (25)) can be derived from (20) by replacing $\hat{x}_k$ with $-\hat{x}_k$ (or from (21) by replacing $\hat{x}_k$ with $-\hat{x}_k$ and $\hat{x}_{N-k}$ with $-\hat{x}_{N-k}$) and exchanging $\sigma_r$ and $\delta_r$ (or exchanging $\hat{\sigma}_r$ and $\hat{\delta}_r$).

Similar to (15), we derive the fully discrete FDM for (17) as: Find $u_i$ such that

$$- \left( \epsilon_1(x_i) L^B_{h,p,q} u + \epsilon_2(x_i) R^B_{h,p,q} \right) + c(x_i) u_i = f(x_i), \quad i = 1, 2, \ldots, N - 1, \quad (28)$$

where $L^B_{h,p,q}$ is defined by (22), $R^B_{h,p,q}$ is defined by (23), and $(p, q) = (1, 0)$ or $(1, -1)$. 

\(\text{(a) } \sigma_k = 0. \quad \text{(b) } \sigma_k = 0.1. \quad \text{(c) } \sigma_k = 0.11. \quad \text{(d) } \sigma_k = 0.1k.\)
4. Numerical results

Simulations to get reliable numerical solutions. In real applications, we will find that even if two correction terms are corresponding results in Tables 2–3. However, we can still apply our method using two correction terms in numerical real parts for \( m \) in Tables 2–3. We observe that for \( \epsilon \) Examples 4.2 and 4.3 in the following; the number of eigenvalues of \( B \) displayed in Table 1. Next, we mainly focus on the eigenvalues of the matrix \( B \) for \( d = 1 \) and \( (\delta_k, \delta_k) = (0.1, 0.9 + 0.1k) \) in \( L^{d \to d} \) for \( i > d \).

Let \( \begin{pmatrix} L B_{h,p,q}^{1,m,d_1} u, \ldots, L B_{h,p,q}^{N-1,m,d_1} u \end{pmatrix} = \frac{1}{\mu} L B_{p,q}^{(a,m,d_1)} u \) and \( \begin{pmatrix} R B_{h,p,q}^{1,m,d_2} u, \ldots, R B_{h,p,q}^{N-1,m,d_2} u \end{pmatrix} = \frac{1}{\mu} R B_{p,q}^{(a,m,d_2)} u \). Then the matrix representation of (28) is

\[
\left( \frac{1}{\mu} B_{p,q}^{a,m,d_1,d_2} + \text{diag}(c) \right) u = f,
\]

(29)

where \( B_{p,q}^{a,m,d_1,d_2} = \text{diag}(\epsilon_1)L B_{p,q}^{(a,m,d_1)} + \text{diag}(\epsilon_2)R B_{p,q}^{(a,m,d_2)} \), \( c = (c(x_1), c(x_2), \ldots, c(x_{N-1}))^T \), and \( \epsilon_r = (\epsilon_r(x_1), \epsilon_r(x_2), \ldots, \epsilon_r(x_{N-1}))^T \), \( r = 1, 2 \).

For \( d_1 = N \) (or \( d_2 = 0 \)), the eigenvalues of the matrix, \( L B_{p,q}^{(a,m,d_1)} \) (or \( R B_{p,q}^{(a,m,d_2)} \)) have similar behavior as the one displayed in Table 1. Next, we mainly focus on the eigenvalues of the matrix \( B_{1,0}^{a,m,d_1,d_2} \) that will be involved in Examples 4.2 and 4.3 in the following; the number of eigenvalues of \( B_{1,0}^{a,m,d_1,d_2} \) with positive real parts is displayed in Tables 2–3. We observe that for \( \epsilon_1 \gg \epsilon_2 \) and \( d_1 = d_2 = N \), all the eigenvalues of \( B_{1,0}^{a,m,d_1,d_2} \) have negative real parts for \( m \leq 6 \) and \( \alpha \leq 1.2 \), see Table 2. For \( d_1 < N \), the result is worse than the case \( d_1 = N \), see the corresponding results in Tables 2–3. However, we can still apply our method using two correction terms in numerical simulations to get reliable numerical solutions. In real applications, we will find that even if two correction terms are used, satisfactory numerical solutions can still be obtained, see numerical results in the following section.

4. Numerical results

In this section, we present several numerical examples to verify our theoretical results by solving two FBVPs and a space-fractional Allen–Cahn equation.

Example 4.1. Consider the following fractional boundary value problem

\[
\begin{align*}
&-\text{RL} D_{0+}^\alpha U(x) + b(x) U'(x) + c(x) U(x) = f(x), \quad x \in (0, 1), \\
&U(0) = 0, \quad U(1) = u_f,
\end{align*}
\]

(30)

where \( 1 < \alpha \leq 2 \), \( b(x), c(x) \geq 0 \).

- Case I: Choose \( b(x) = 0 \), \( b(x) = 1 \), \( u_f = 2 \), and a suitable force term \( f(x) \) such that the analytical solution of (30) is \( U(x) = (x^{\alpha-1} + x^{1+\alpha} + x^{2+\alpha})/2 \).
- Case II (comparison with the Petrov–Galerkin finite element method in [43]): Choose \( b(x) = e^x \), \( c(x) = x(1 - x) \), \( u_f = 0 \), and the force term \( f(x) = x \) or \( f(x) = 1 \).
- Case III: Choose \( b(x) = 0 \), \( c(x) = 1 \), \( u_f = 2 \), and the force term \( f(x) = \sin(\pi x) \).
- Case IV (comparison with the linear finite element method in [18]): Solve (30) subject to the homogeneous boundary conditions with \( b(x) = 0 \), \( c(x) = x \), and \( f(x) = 1 \).
The $L^\infty$ error $\|e\|_\infty$ and $L^2$ error $\|e\|$ for Example 4.1, Case I, $\alpha = 1.1$, and $(p, q) = (1, 0)$.

<table>
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<tr>
<th>$N$</th>
<th>$m = 0$</th>
<th>$m = 1$</th>
<th>$m = 2$</th>
<th>$m = 3$</th>
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<td>$L^\infty$ error</td>
<td>$L^\infty$ error</td>
<td>$L^\infty$ error</td>
<td>$L^\infty$ error</td>
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<tr>
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<tr>
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<tr>
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<tr>
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</tr>
<tr>
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<td>1.5049e−5</td>
<td>1.0641e−5</td>
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</tbody>
</table>

The $L^2$ error $\|e\|$ and the $L^\infty$ error $\|e\|_\infty$ are measured in the following sense

$$\|e\| = \sqrt{\frac{1}{h} \sum_{j=0}^{N-1} (U(x_j) - u_j)^2}, \quad \|e\|_\infty = \max_{0 \leq j \leq N} |U(x_j) - u_j|.$$ 

We employ the method (15) with and without correction terms to solve (30).

For Case I, the analytical solution is known and this kind of solution is chosen in order to mimic the real behavior of the analytical solution to the considered FDEs. Hence, we can set $\sigma_k = k - 2 + \alpha$ in numerical simulations. Tables 4–6 display the $L^2$ errors and the $L^\infty$ errors for different fractional orders $\alpha = 1.1, 1.5, 1.9$. We can see that second-order accuracy is observed for both $L^2$ errors and $L^\infty$ errors when the number of correction terms $m = 2, 3$, which is inline with the theoretical analysis, see (14). We also observe that the $L^2$ error shows better behavior than the maximum error. Specially, we observe from Table 4 that very low accuracy is achieved without correction terms. Obviously, adding suitable correction terms increases the accuracy significantly whether the regularity of the analytical solution is low or not, which will be further demonstrated in Cases II–IV in this example.

For Case II, we do not have analytical solutions. However, the analytical solution contains the low order term $x^{(\alpha-1)}$, see Theorem 4.8 and Section 5 in [43]. Hence, we choose $m = 1, 3$ and let $\sigma_1 = \alpha - 1, \sigma_2 = 1, \sigma_3 = 2(\alpha - 1)$ in (15), the $L^2$ errors are shown in Tables 7 and 8. We can see that the FDM (15) achieves better numerical solutions even with one correction term.
The $L^\infty$ error $\|e\|^\infty_\infty$ and $L^2$ error $\|e\|$ for Example 4.1, $\alpha = 1.9$, and $(p, q) = (1, 0)$.

<table>
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<th>$L^\infty$ error</th>
<th>Order</th>
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<th>Order</th>
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Comparison of the $L^2$ errors between the FDM (15) with $(p, q) = (1, 0)$ and the PGFEM (see Table 3 in [43]) for Case II, $f(x) = x$, $\sigma_1 = \alpha - 1$, $\sigma_2 = 1$, $\sigma_3 = 2(\alpha - 1)$. The reference solutions are obtained with $N = 2560$.

<table>
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Comparison of the $L^2$ errors between the FDM (15) with $(p, q) = (1, 0)$ and the PGFEM (see Table 6 in [43]) for Case II, $f(x) = x$, $\sigma_1 = \alpha - 1$, $\sigma_2 = 1$, $\sigma_3 = 2(\alpha - 1)$. The reference solutions are obtained with $N = 2560$.

<table>
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<tr>
<th>$N$</th>
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<td>5.34e-5</td>
<td>5.78e-4</td>
<td>4.42e-5</td>
<td>1.41e-5</td>
</tr>
<tr>
<td>160</td>
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<td>2.65e-4</td>
<td>1.32e-5</td>
<td>3.48e-6</td>
</tr>
<tr>
<td>320</td>
<td>1.32e-5</td>
<td>3.38e-6</td>
<td>1.22e-4</td>
<td>3.89e-6</td>
<td>8.57e-7</td>
</tr>
</tbody>
</table>

For Case III, we have only the source term $f(x)$ and the analytical solution is unknown. However, we know the regularity of the solution, which contains the low-order term $x^{(\alpha - 1)}$ when $\alpha$ is sufficiently small, see [5]. Hence, we first set $\sigma_k = k(\alpha - 1)$ in the computation, and the numerical solutions are shown in Fig. 4.1(a). We can see that wiggles appear when no correction term is employed, but disappear when suitable correction terms are added. In real applications, we may not know the regularity (or singularity) index of the analytical solution of the considered FDEs, i.e., non-linear FDEs. We will show that our method is still effective by choosing suitable correction terms. Here, we choose $\sigma_k = k(\alpha - 1) + 0.11$ that does not match the regularity index of the analytical solution; the numerical solutions are shown in Fig. 4.1(b). We find that very satisfactory numerical solutions are obtained as the number of “correction terms” increases. This can be explained from the small coefficient $S_{\sigma} = \prod_{k=1}^{m} |\sigma_k - \sigma|$ in the error bound (12), where $\sigma = \alpha - 1$ in Case III that determines the convergence of the method (15). This positive effect on the accuracy improvement of numerical solutions will be further demonstrated in the following examples by solving a
of the analytical solutions. FDE with two-sided fractional derivatives and a fractional Allen–Cahn equation, where we do not know the regularity of the reference solutions are obtained with the maximum error, which is inline with the theoretical analysis. In fact, numerical solutions have wiggles near the second-order accuracy is observed as the number of correction terms increases and the average error is better than the errors between the FDM (15) with and a suitable force term that makes the method (28) exact for low regularity terms. We first choose a Case I: Choose \( \varepsilon_1 = \varepsilon_2 = 1 \) and a suitable force term \( f(x) \) such that the analytical solution of (31) is 
\[
U(x) = x^\alpha - (1 - x)^{\alpha - 1} + x\alpha(1 - x)\alpha + x^2 + (1 - x)^{2 + \alpha}.
\]
• Case II: Choose a force term \( f(x) = 1 + \sin(5x) \) and 
(A) \( \varepsilon_1 = \varepsilon_2 = 1, \alpha = 1.1, 1.2, 1.3, 1.5, 1.8 \) without correction terms; 
(B) \( \varepsilon_1 = 6, \varepsilon_2 = 1, \alpha = 1.1, 1.2, 1.3, 1.5, 1.8 \) without correction terms; 
(C) \( \varepsilon_1 = 6, \varepsilon_2 = 1, \alpha = 1.05, 1.1 \) with correction terms; 
(D) \( \varepsilon_1 = 1, \varepsilon_2 = 6, \alpha = 1.05, 1.1 \) with correction terms.

For Case I, we first set \( (d_1, d_2) = (N, 0) \) in (28). Since we know the exact solution, one good choice is \( \sigma_k = \delta_k = \hat{\sigma}_k = \hat{\delta}_k = \alpha - 2 + k \) that makes the method (28) exact for low regularity terms. We first choose a relatively smaller fractional order \( \alpha = 1.1 \); the \( L^\infty \) errors and the \( L^2 \) errors are shown in Table 10. We can see that second-order accuracy is observed as the number of correction terms increases and the average error is better than the maximum error, which is inline with the theoretical analysis. In fact, numerical solutions have wiggles near the

Table 9
Comparison of the \( L^2 \) errors between the FDM (15) with \( (p, q) = (1, 0) \) and the linear FEM (see Table 3 in [18]) for Case IV, \( \sigma_k = k(\alpha - 1) \). The reference solutions are obtained with \( N = 2048 \).

<table>
<thead>
<tr>
<th>( N )</th>
<th>( \alpha = 1.05 )</th>
<th>( \alpha = 1.25 )</th>
<th>( \alpha = 1.45 )</th>
</tr>
</thead>
<tbody>
<tr>
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<td>( m = 5 )</td>
<td>( m = 3 )</td>
<td>( m = 5 )</td>
</tr>
<tr>
<td>( 8 )</td>
<td>2.08e–3</td>
<td>3.78e–3</td>
<td>5.13e–2</td>
</tr>
<tr>
<td>( 16 )</td>
<td>7.84e–4</td>
<td>5.74e–4</td>
<td>3.12e–2</td>
</tr>
<tr>
<td>( 32 )</td>
<td>3.10e–4</td>
<td>1.81e–4</td>
<td>1.73e–2</td>
</tr>
<tr>
<td>( 64 )</td>
<td>1.14e–4</td>
<td>7.13e–5</td>
<td>8.97e–3</td>
</tr>
<tr>
<td>( 128 )</td>
<td>4.05e–5</td>
<td>2.70e–5</td>
<td>4.41e–3</td>
</tr>
<tr>
<td>( 256 )</td>
<td>1.40e–5</td>
<td>9.65e–6</td>
<td>2.06e–3</td>
</tr>
</tbody>
</table>

FDE with two-sided fractional derivatives and a fractional Allen–Cahn equation, where we do not know the regularity of the analytical solutions.

At last in Case IV, we compare our method with the FEM developed in [18]; the \( L^2 \) errors are displayed in Table 9. We can see that the present method with suitable correction terms shows much better accuracy, even for the very small fractional order that leads to stronger singularity.

Example 4.2. Consider the following one-dimensional fractional boundary value problem

\[
\begin{cases}
-\left( \varepsilon_1 \operatorname{RLD}_{0,x}^{\alpha} + \varepsilon_2 \operatorname{RLD}_{1}^{\alpha} \right) U(x) + U(x) = f(x), & x \in (0, 1), \\
U(0) = 0, & U(1) = 0,
\end{cases}
\]

(31)

where \( 1 < \alpha \leq 2 \), \( \varepsilon_1, \varepsilon_2 \geq 0 \), and \( \varepsilon_1^2 + \varepsilon_2^2 \neq 0 \).

• Case I: Choose \( \varepsilon_1 = \varepsilon_2 = 1 \) and a suitable force term \( f(x) \) such that the analytical solution of (31) is 
\[
U(x) = x^\alpha - (1 - x)^{\alpha - 1} + x\alpha(1 - x)^\alpha + x^{1+\alpha}(1 - x)\alpha + x^{2+\alpha}(1 - x)^{2+\alpha}.
\]

• Case II: Choose a force term \( f(x) = 1 + \sin(5x) \) and

(A) \( \varepsilon_1 = \varepsilon_2 = 1, \alpha = 1.1, 1.2, 1.3, 1.5, 1.8 \) without correction terms;

(B) \( \varepsilon_1 = 6, \varepsilon_2 = 1, \alpha = 1.1, 1.2, 1.3, 1.5, 1.8 \) without correction terms;

(C) \( \varepsilon_1 = 6, \varepsilon_2 = 1, \alpha = 1.05, 1.1 \) with correction terms;

(D) \( \varepsilon_1 = 1, \varepsilon_2 = 6, \alpha = 1.05, 1.1 \) with correction terms.

Fig. 4.1. Numerical solutions for Case III, \( \alpha = 1.1 \), \( N = 128 \), and \( (p, q) = (1, 0) \).
are obtained without correction terms due to the relatively good regularity of the analytical solutions. While for Case II, we do not have the explicit form of the analytical solutions. We mainly investigate the FBVP (31) with fractional order \( \alpha \) from the small coefficient \( S \) of numerical solutions is obviously improved as the number of correction terms \( \delta_k \) increases for \( k \geq 1 \).

Next, we focus on how the correction terms affect the accuracy of the present method. Here we still consider Case I and set \( \alpha = 1.1, (d_1, d_2) = ([N/2], [N/2]) \), \( N = 256 \), and \( (p, q) = (1, 0) \). Let \( \delta_k = \hat{\delta}_k = 0 \), and \( \delta_k = k/10 + \epsilon \), \( k \geq 1 \).

Table 10 shows first numerical results for Case II (A) in Fig. 4.2(a) and observe that relatively good numerical solutions are obtained without correction terms due to the relatively good regularity of the analytical solutions. While for Case II (B), we observe wiggles near the left end-point when \( \alpha \to 1 \) and \( \epsilon_1/\epsilon_2 = 6 > 1 \), see \( \alpha = 1.1, 1.2 \) in Fig. 4.2(b). As

<table>
<thead>
<tr>
<th>( N )</th>
<th>( L^\infty ) error</th>
<th>( L^2 ) error</th>
<th>( L^\infty ) error</th>
<th>( L^2 ) error</th>
<th>( L^\infty ) error</th>
<th>( L^2 ) error</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>1.1863e-1</td>
<td>1.6831e-2</td>
<td>5.6984e-3</td>
<td>1.1116e-3</td>
<td>2.0981e-4</td>
<td>2.4054</td>
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<tr>
<td>20</td>
<td>1.3077e-1</td>
<td>9.3115e-3</td>
<td>1.6310e-3</td>
<td>1.8048</td>
<td>3.1687e-5</td>
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</tr>
<tr>
<td>40</td>
<td>1.3628e-1</td>
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</tr>
<tr>
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<td>0.0414</td>
<td>2.5994e-5</td>
<td>2.0401</td>
<td>1.4394e-6</td>
<td>1.9121</td>
</tr>
</tbody>
</table>

Table 11 shows the L∞ error (upper) and L2 error (down) for Example 4.2, Case I, \( \alpha = 1.1, (d_1, d_2) = ([N/2], [N/2]), N = 256, (p, q) = (1, 0), \( \delta_k = \hat{\delta}_k = 0 \), and \( \delta_k = k/10 + \epsilon \), \( k \geq 1 \).

<table>
<thead>
<tr>
<th>( \epsilon )</th>
<th>( m = 0 )</th>
<th>( m = 1 )</th>
<th>( m = 2 )</th>
<th>( m = 3 )</th>
<th>( m = 4 )</th>
<th>( m = 5 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00</td>
<td>1.2843e-1</td>
<td>7.9307e-2</td>
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<tr>
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</tr>
<tr>
<td>0.03</td>
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<td>4.7448e-2</td>
<td>8.5196e-4</td>
<td>1.2169</td>
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<tr>
<td>0.04</td>
<td>1.2843e-1</td>
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<td>1.3773</td>
<td>9.1605e-7</td>
<td>1.8174</td>
</tr>
</tbody>
</table>

For Case II, we do not have the explicit form of the analytical solutions. We mainly investigate the FBVP (31) with fractional order \( \alpha \) being close to one. In such a case, the analytical solution has stronger singularity at the left (or right) end-point when \( \epsilon_1/\epsilon_2 \gg 1 \) (or \( \epsilon_1/\epsilon_2 \ll 1 \), see [27]. Due to the symmetry of the Riesz fractional derivative operator, the analytical solution of (31) has relatively good regularity if \( \epsilon_1 = \epsilon_2 \); see related results in [46,21,27].

We show first numerical results for Case II (A) in Fig. 4.2(a) and observe that relatively good numerical solutions are obtained without correction terms due to the relatively good regularity of the analytical solutions. While for Case II (B), we observe wiggles near the left end-point when \( \alpha \to 1 \) and \( \epsilon_1/\epsilon_2 = 6 > 1 \), see \( \alpha = 1.1, 1.2 \) in Fig. 4.2(b). As
Table 12
The $L^\infty$ error (upper) and $L^2$ error (down) for Example 4.2, Case I, $\alpha = 1.1$, $(d_1, d_2) = ([N/2], [N/2])$, $N = 256$, $(p, q) = (1, 0)$, $\delta_k = \delta_k = \alpha - 1$, and $\delta_k = \sigma_k = k/10 + \epsilon$, $k \geq 1$.

<table>
<thead>
<tr>
<th>$\epsilon$</th>
<th>$m = 0$</th>
<th>$m = 1$</th>
<th>$m = 2$</th>
<th>$m = 3$</th>
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<tbody>
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<td>1.2105e-3</td>
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<tr>
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<td>2.8923e-2</td>
<td>1.1301e-2</td>
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<td>2.0491e-3</td>
<td>1.0187e-3</td>
<td>6.4090e-4</td>
</tr>
</tbody>
</table>

(a) Case II (A), $\varepsilon_1 = \varepsilon_2 = 1$.
(b) Case II (B), $\varepsilon_1 = 6$, $\varepsilon_2 = 1$.

Fig. 4.2. Numerical solutions for Cases II (A) and II (B), $N = 128$, $m = 0$ and $(p, q) = (1, 0)$.

the fractional order $\alpha$ increases, wiggles disappear due to the relatively good regularity of the analytical solution, see $\alpha = 1.3, 1.5, 1.8$ in Fig. 4.2(b). Next, we focus on the good performance of the present method using the correction terms that significantly enhance the accuracy of the numerical solutions when the analytical solution has stronger singularity at the end-point(s).

For Case II (C), the solution has stronger singularity at the left-end point, i.e., the solution contains $x^\sigma (1 - x)^\delta$ and $\sigma$ is relatively small while $\delta$ is relatively large. (i) We first let $d_1 = d_2 = N$ and set $\sigma_k = \hat{\sigma}_k = k(\alpha - 1)$ and $\delta_k = \hat{\delta}_k = 1 + 0.1k (k \geq 1)$ in (28); numerical solutions for $\alpha = 1.05, 1.1$ are displayed in Fig. 4.3. We can see that the modified WSGL formula with suitable correction terms achieves better numerical solutions than the standard WSGL formula. (ii) The parameters are chosen the same as (i), except that $(d_1, d_2) = ([7N/8], [N/8])$, where $\sigma_k = k(\alpha - 1)$, $\hat{\sigma}_k = 0$, and $\hat{\delta}_k = 1 + k(\alpha - 1)$ in both $L_{h,p,q}^{\delta,i,m,d}$ and $R_{h,p,q}^{\delta,i,m,d}$; numerical solutions are displayed in Fig. 4.4. We can see that very good results are still obtained, which may be explained from the results in Fig. 3.3.

Similar results are shown in Fig. 4.5, where the analytical solution has stronger singularity at the right end-point for Case II (D). Here, we choose $d_1 = d_2 = 0$, $\sigma_k = \hat{\sigma}_k = 1 + 0.1k (k \geq 1)$, and $\delta_k = \hat{\delta}_k = k(\alpha - 1)$ in the computation. We observe that the present method produces better results than the standard WSGL formula (see $m = 0$ in Fig. 4.5). We refer the readers to [27] for more related results. We can also choose other parameters of $(d_1, d_2) = ([7N/8], [N/8])$ and $\sigma_k = k(\alpha - 1)$, $\hat{\sigma}_k = 1 + k(\alpha - 1)$, $\hat{\delta}_k = \delta_k = 0$ yields similar results as displayed in Fig. 4.5, which are not provided here.
Example 4.3. Consider the following space-fractional Allen–Cahn equation

\[
\begin{align*}
\partial_t U &= \left( \epsilon_1 RL D_{-1,x}^\alpha + \epsilon_2 RL D_{x,1}^\alpha \right) U + U(1 - U^2), \\
U(x, 0) &= \phi(x), \\
U(-1, t) &= U(1, t) = 0
\end{align*}
\]

where \( 1 < \alpha \leq 2, \epsilon_1, \epsilon_2 \geq 0 \) are constants, \( \epsilon_1^2 + \epsilon_2^2 \neq 0 \), and \((x, t) \in (-1, 1) \times (0, T), T > 0\).

We apply the second-order semi-implicit time discretization in time to solve (32). Let \( \tau \) be the time stepsize with \( \tau = T/n_T, n_T \) is a positive integer, and \( t_n = n \tau \). The fully discrete FDM for (32) is given as: Find \( u^n_i \) \((1 \leq n \leq n_T - 1, 1 \leq i \leq N - 1)\), such that

\[
\begin{align*}
3u_i^{n+1} - 4u_i^n + u_i^{n-1} &= \frac{2\tau}{\epsilon_1 L B_{h,p,q}^{\alpha,i,m,d_1} + \epsilon_2 R B_{h,p,q}^{\alpha,i,m,d_2}} u_i^{n+1} + (2F_i^n - F_i^{n-1}), \\
u_i^0 &= \phi(x_i), \\
u_i^1 &= u_i^0 + \tau \partial_t U(x_i, 0), \quad i = 0, 1, \ldots, N, \\
u_i^n &= u_i^{n-1} = 0, \quad n = 0, 1, \ldots, n_T,
\end{align*}
\]

where \( F_i^n = F(u_i^n) = u_i^n - (u_i^n)^3 \).
The following cases will be considered in the numerical simulations.

- Case I: Let \((\epsilon_1, \epsilon_2) = (0.5, 0.5)\) or \((0.9, 0.1)\) for \(\alpha = 1.05, 1.1, 1.2, 1.3, 1.4\) in the computation without correction terms;
- Case II: Let \((\epsilon_1, \epsilon_2) = (0.9, 0.1)\), \((d_1, d_2) = (N, 7\lceil N/8 \rceil)\) for \(\alpha = 1.05, 1.1\);
- Case III: Let \((\epsilon_1, \epsilon_2) = (0.1, 0.9)\), \((d_1, d_2) = (\lceil N/8 \rceil, 0)\) for \(\alpha = 1.05, 1.1\).

In the numerical simulations in the following, we always choose the initial condition \(\phi(x) = \sin(\pi x)\), \((p, q) = (1, 0)\), and \(N = 128\) in the method (33). Unlike the previous two examples, the regularity of the analytical solution in this example also depends on time \(t\). We will show that our method still works well.

We first consider Case I by applying the method (33) without correction terms; numerical solutions at \(t = 0.4\) are displayed in Fig. 4.6 for different fractional orders \(\alpha = 1.05, 1.1, 1.2, 1.3, 1.4\). We observe that relatively good numerical solutions are obtained (see Fig. 4.6(a)) when choosing \(\epsilon_1 = \epsilon_2 = 0.5\), due to the relatively good regularity of the analytical solutions. However, wiggles appear near the left end-point when choosing \(\epsilon_1 = 0.9 > 0.1 = \epsilon_2\) due to the stronger singularity for small fractional order, see Fig. 4.6(b) with \(\alpha = 1.05, 1.1, 1.2\). As the fractional order \(\alpha\) increases, wiggles disappear due to the relatively good regularity of the analytical solutions, see Fig. 4.6(b) with \(\alpha = 1.3, 1.4\). This coincides with the numerical results in the previous example, see also related results in [27].

For Cases II and III, we are concerned with small fractional order that may lead to stronger singularity of the analytical solution and show the effectiveness of the present method.

We still choose \(\epsilon_1 = 0.9\) and \(\epsilon_2 = 0.1\) in Case II. Other parameters in (33) are chosen as \(\sigma_k = 0.1k, \hat{\delta}_k = 0.9 + 0.1k, \delta_k = \hat{\alpha}k = 0\), and \((d_1, d_2) = (N, 7\lceil N/8 \rceil)\). Numerical solutions for \(\alpha = 1.05\) and \(\alpha = 1.1\) at \(t = 0.4\) are displayed in Fig. 4.7. We can see that wiggles disappear as the number of “correction terms” increases.

From all the previous numerical results in this work, we can find that two “correction terms” are enough to get satisfactory numerical solutions. It is also safe to use less than two correction terms to guarantee the stability of (33), see also Tables 2–3. We still consider Case II and the parameters in (33) are chosen the same as Fig. 4.7 except for \((d_1, d_2) = (\lceil N/2 \rceil, \lceil N/2 \rceil)\); numerical solutions for \(\alpha = 1.1\) at \(t = 0.4, 0.8, 1, 2\) are displayed in Fig. 4.8. We can see that the singularity really changes with time, becoming much stronger causing inaccurate numerical solutions using the original WSGL formula, see \(m = 0\) in Fig. 4.8. However, the new formula with one or two correction terms shows much more accurate numerical solutions, see \(m = 1, 2\) in Fig. 4.8.

For Case III, similar behavior is observed in Fig. 4.9, where the analytical solution has stronger singularity at the right end-point. Here, we choose \(\sigma_k = 0.9 + 0.1k, \quad \delta_k = 0.1k, \quad \delta_k = 0\), \((d_1, d_2) = (\lceil N/8 \rceil, 0)\) in the computation. We observe that numerical solutions become better by tuning the correction terms. We can also choose other \((d_1, d_2)\) with one or two correction terms in the computation, i.e., \((d_1, d_2) = (\lceil N/2 \rceil, \lceil N/2 \rceil)\); satisfactory numerical solutions can be obtained, although the detailed results are not shown here.
Fig. 4.6. Numerical solutions at $t = 0.4$ for Case I, $m = 0$, and $N = 128$.

Fig. 4.7. Numerical solutions at $t = 0.4$ for Case II, $\epsilon_1 = 0.9$, $\epsilon_2 = 0.1$, $(d_1, d_2) = (N, 7\lceil N/8 \rceil)$, and $N = 128$.

5. Summary

In this paper, we proposed a tunable finite difference method by using the second-order accurate WSGL formulas with correction terms to solve fractional boundary value problems and FPDEs with two end-point singularities.

We show theoretically and numerically that the original second-order WSGL formula [41] does not exhibit global second-order accuracy for approximating the left (or right) RL fractional derivative, even if the functions are sufficiently smooth, see Fig. 2.1. In order to overcome this drawback, we follow Lubich’s approach [36] to introduce suitable correction terms into the original WSGL formula and derive the modified WSGL formula, which preserves second-order accuracy.

We note that the correction terms are chosen such that the derived method is exact for the low regularity part of the solutions and leads to high-order accuracy for the high regularity part of the solutions, see [36]. We need to know the regularity index of the solutions, which may be difficult to know. However, we find that the correction indices do not need to coincide with the low regularity indices of the analytical solutions; high accuracy can still be preserved thanks to the small coefficient in the error equation of the new discretization method, see Lemma 2.2, Eq. (12), and numerical results displayed in Fig. 2.2; see also related results in [40].

One concern is that the coefficient matrix from the modified WSGL formula may have zero or nearly zero eigenvalues when the number of correction terms is large (see Tables 1–3), which may lead to unstable numerical schemes when applied to solve the time-dependent FDEs. Numerical simulations show that our method works well using only a very small number of correction terms and satisfactory numerical solutions are obtained.
In the future, we will explore how to add correction terms that can make the new discretization more robust with the coefficient matrix resulted from the new discretization guaranteed to be negative definite. We will also extend the hybrid formulas we introduced (see Eqs. (22) and (23)) to relate the switchover point \(d\) to the values of the coefficients \(\epsilon_1\) and \(\epsilon_2\). Alternatively, we may explore other ways to add correction terms, see for example [47]. The present

![Graphs](image-url)
approach can be extended to solve high dimensional FDEs, even more general singular integral equations and the classical equations with singularities.

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References