

Article

A Concise Review on the Numerical Treatment of Generalized Fractional Equations

Xuhao Li ¹ and Patricia J. Y. Wong ^{2,*} ¹ School of Mathematical Sciences, Anhui University, Jiulong Road, Hefei 230601, China; lixh@ahu.edu.cn² School of Electrical and Electronic Engineering, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798, Singapore

* Correspondence: ejywong@ntu.edu.sg

Abstract

In this paper, we shall give a concise review of recent numerical methods of some generalized fractional models. As is elucidated later, the generalized fractional models may arise from either mathematical point of view or application point of view. We shall focus on the former one and discuss the numerical methods for these models in a concise manner. Finally, some potential research directions are proposed based on existing results as well as some advanced new topics. We hope this review can provide a sketch of current and future studies of generalized fractional models for interested readers.

Keywords: generalized fractional model; time-diffusion problem; generalized interpolation; generalized convolution quadrature

MSC: 65M12; 65M22

1. Introduction

Generally speaking, models involving fractional operators are called fractional models in the literature. Fractional models have been shown to be useful and necessary in engineering [1,2], biochemistry [3,4], physics [5,6], statistical physics [3,4,7], statistical mechanics [8] and other disciplines [2,6,9]. More recently, Noeiaghdam and Sidorov [10] found that fractional models are superior to classical models in energy supply–demand systems, which enhances the application of fractional models. The fractional operators or fractional calculus may originate from a letter of L'Hospital to Leibniz in 1695 [11]. An intriguing problem incurred from that letter is the meaning of non-integer order integral or derivative. Many well known mathematicians like Fourier, Euler, Laplace, Lagrange, Liouville, Riemann, Gröwald, Letnikov and Caputo [1,2,12,13] have tried to give a proper definition in their own ways and thus have contributed to the gradual development of fractional calculus. Nowadays, it is known that Riemann-Liouville's and Caputo's definitions [1,2] are widely adopted in time fractional models as they are closely related to memory processes that are prevalent in nature. These fractional operators can also be used to characterize spatial relations and thus lead to space fractional models, for example Riesz fractional derivative [14,15], which combines left and right Riemann-Liouville fractional derivatives. However, the use of Riemann-Liouville and Caputo fractional derivatives is mostly limited to one-dimensional problems. For high-dimensional problems, a more natural choice is the fractional Laplacian, which is beyond the scope of this work; interested readers can refer to the excellent review paper [16] and the references therein.



Academic Editors: Giuseppe Di Fazio and Luigi Rodino

Received: 20 June 2025

Revised: 31 October 2025

Accepted: 10 November 2025

Published: 19 November 2025

Citation: Li, X.; Wong, P.J.Y.

A Concise Review on the Numerical Treatment of Generalized Fractional Equations. *Mathematics* **2025**, *13*, 3713. <https://doi.org/10.3390/math13223713>

Copyright: © 2025 by the authors.

Licensee MDPI, Basel, Switzerland.

This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<https://creativecommons.org/licenses/by/4.0/>).

There are at least two ways to derive fractional models. One way is to replace integer order operators by fractional ones. It is simple and straightforward but may not easily convince scientists of its practical values. Another way is to model phenomena arising from physics or biochemistry at the macroscopic level or microscopic level [3,4,7,17]. The former may rely on some empirical laws that also need to be proven, while the latter applies stochastic processes, and the probability density function of statistical observables of the stochastic processes naturally satisfy some fractional models. Once the fractional models are derived, one can analyze their properties (e.g., well-posedness, regularity) and construct numerical methods of these models. In fact, these topics have been discussed and investigated extensively in recent decades; see [18,19] for well-posedness and regularities of initial boundary value problems for fractional diffusion equations, [17] for wellposedness of fractional and tempered fractional problems, [14] for weighted convolution quadrature method of space diffusion problem, [15] for Riesz basis spectral Galerkin method of tempered fractional Laplacian, [20] for time discretization of tempered fractional Feymann-Kac equations, [21] for stochastic fractional models, [3] for a thorough review regarding time fractional and space fractional problems, [22,23] for L1 method and convolution quadrature method of fractional diffusion equation with nonsmooth data, [24] for Crank-Nicolson method of fractional subdiffusion equation, [25] for convolution quadrature method of nonlinear fractional subdiffusion problem, [26,27] for L1 method with uniform and graded mesh for fractional subdiffusion equation, and [28] for adaptive-coefficient finite difference frequency domain method for the time fractional diffusive-viscous wave equation, and the references therein. In this review, we mainly focus on the numerical methods of the time fractional models.

Typically, there are two types of numerical methods, namely the **interpolation method** and **convolution quadrature method**, that are widely used in solving time fractional problems. The main idea of the **interpolation method** lies in that the integrand function is approximated by interpolation at discrete pairs of nodes. In fact, one will achieve the L1 type method [27,29–32] and L2 type method [33–41] if piecewise linear interpolation and piecewise quadratic interpolation are applied, respectively. It is known that L1 and L2 type methods can only give $2 - \alpha$ and $3 - \alpha$ ($0 < \alpha < 1$) orders of accuracy, respectively. High-order methods [42,43] can be similarly constructed using high-order interpolations, but the analysis of the resulting numerical scheme is known to be challenging. Additionally, when the analytical solution of the model has singularity, which is a common situation in applications [19,26], L1 and L2 type methods will reduce to first-order accuracy if the uniform mesh is applied. To tackle this problem, an efficient and popular technique is to adopt an interpolation method with non-uniform mesh, such as graded mesh [27,37], quasi graded mesh [30] or more general mesh [31,36,40,44].

In addition to the interpolation method described above, there is the **convolution quadrature method**, which originates from Lubich [45–48]. This method is the first method proposed to approximate the convolution of the given singular kernel $t^{\alpha-1}$ and a function that has singularity at $t = 0$, and the integer order derivative of this convolution is exactly the Riemann-Liouville fractional derivative. This method has a close relation to a linear multistep method called the k -th backward difference formula (or BDFk [49]). Actually, the generating function of the convolution quadrature method is a fractional power of the generating function of the related BDFk method. It is also shown in [50] that the convolution quadrature method is promising in tackling fractional problems. After that, it is well developed by Jin and his collaborators [22,23,25,29] to solve time fractional problems by incorporating initial corrections. Compared to the interpolation method, the convolution quadrature method can obtain k -th order accuracy that is better than the interpolation method if $k \geq 3$, and the method may be analyzed in a general framework.

However, the convolution quadrature method requires the uniform mesh and can only obtain at most sixth-order accuracy as BDFk method is unstable if $k > 6$, see [23,45,49]. In recent years, there has been some remarkable progress in the variable-step BDFk ($k \leq 3$) method [51–55] that can work for non-uniform mesh. Hopefully, it may be extended to solve fractional problems and thus the computation cost may be further significantly reduced. On the other hand, it is found that a linear combination of the fractional BDF1 method (or equivalently Grünwald-Letnikov method) can obtain second-order accuracy, which improves the pure fractional BDF1 that has only first-order accuracy. This method is known as **weighted shifted Grünwald-Letnikov (WSGL) method** [56]; see [14,57] for some recent developments with seven steps and four steps, respectively. This opens new possibilities for a higher-accuracy method based on the convolution quadrature method.

Recently, some **generalized fractional operators** [4,58–60] have been proposed and applied to model natural phenomena more accurately. In what follows, we shall introduce the generalized fractional models from two perspectives in Section 2. Then, some existing numerical methods for certain generalized fractional problems are presented concisely in Section 3. Section 4 illustrates the numerical performance and convergence of the numerical schemes presented in Section 3. Thereafter, in Section 5, some potential research directions are proposed based on our discussions and new developments. Finally, we end this paper with a summary in Section 6.

2. Generalized Fractional Models

In this section, we shall first present the basics of fractional derivatives before introducing some generalized fractional models from two perspectives: mathematical and application.

2.1. Fractional Derivative

Let $a < b$. Denote $C^n[a, b]$ as the space of functions that have continuous derivatives up to n , $L^p[a, b]$ ($p \geq 1$) as the standard space of Lebesgue integrable functions over $[a, b]$ such that $\int_a^b |f(t)|^p dt < \infty$, $AC[a, b]$ as the space of functions that are absolutely continuous, and $AC^n[a, b]$ as the space of functions which have continuous derivatives up to $n - 1$ with $f^{(n-1)}(t) \in AC[a, b]$. Obviously, we have $AC^1[a, b] = AC[a, b]$. Furthermore, let $D_t^m := \frac{d^m}{dt^m}$.

Recall that the classical fractional integral [1,2] is defined as follows.

Definition 1. Let $\alpha > 0$ be a real number. For $f \in L^1[a, b]$, the classical fractional integral of $f(t)$ is defined as

$${}_a I_t^\alpha f(t) = \frac{1}{\Gamma(\alpha)} \int_a^t (t-s)^{\alpha-1} f(s) ds.$$

Let $m = \lceil \alpha \rceil$ ($\alpha > 0$). Combining Definition 1 with D_t^m , the α -th order Riemann-Liouville (RL) fractional derivative and Caputo fractional derivative can be readily given. Specifically, we have the following definition (see [1,61]).

Definition 2.

- (RL) Let $f(t) \in AC^m[a, b]$. The following α -th order Riemann-Liouville fractional derivative

$${}_a D_t^\alpha f(t) = D_t^m ({}_a I_t^{m-\alpha} f(t)),$$

exists almost everywhere. If we further have $({}_a I_t^{m-\alpha} f(t)) \in C^m[a, b]$, then it is well defined in the classical sense.

- (Caputo) Let $D_t^m f(t) = f^{(m)}(t) \in L^1[a, b]$. Then, we can define the α -th order Caputo fractional derivative as

$${}_a^C D_t^\alpha f(t) = {}_a I_t^{m-\alpha} (D_t^m f(t)).$$

The fractional derivatives presented in Definition 2 are widely used to model memory effects in engineering, biochemistry, and statistical physics in the literature. In what follows, we shall introduce the generalized operators of the aforementioned classical fractional derivatives. We note that there are alternative ways to define fractional integrals or derivatives, e.g., Hadamard fractional operator [61,62], defined as follows

$$D_+^\alpha f(t) = \frac{\beta}{\Gamma(1-\beta)} \int_0^t (\ln(t) - \ln(s))^{-1-\beta} \frac{f(t) - f(s)}{s} ds;$$

conformable fractional derivative [63,64] that is defined as

$$T_\beta(f)(t) = \lim_{\epsilon \rightarrow 0} \frac{f(t + \epsilon t^{1-\beta}) - f(t)}{\epsilon}, \quad t > 0;$$

and β conformable fractional derivative [65], which is an extension of conformable fractional derivative, defined as

$$MT_\beta(f)(t) = \lim_{\epsilon \rightarrow 0} \frac{f(t + \epsilon(t + 1/\Gamma(\beta))^{1-\beta}) - f(t)}{\epsilon}, \quad t > 0,$$

where $\beta \in (0, 1)$. Moreover, there is more than one way to generalize them based on Definitions 1 and 2. For example, Erdélyi-Kober fractional derivative that arises from stochastic process driven by generalized grey Brownian motion instead of Brownian motion [66–70]. It is defined as

$$D_\eta^{\gamma, \alpha} f(t) = \prod_{j=1}^m \left(\gamma + j + \frac{1}{\eta} t D_t \right) I_\eta^{\gamma + \alpha, m - \alpha} f(t),$$

where $\eta > 0$, $\gamma \in \mathbb{R}$ and $I_\eta^{\gamma + \alpha, m - \alpha} f(t)$ is Erdélyi-Kober fractional integral given by

$$I_\eta^{\gamma + \alpha, m - \alpha} f(t) = \frac{\eta t^{-\eta(\alpha + \gamma)}}{\Gamma(\alpha)} \int_a^t s^{\eta(\gamma + 1) - 1} (t^\eta - s^\eta)^{\alpha - 1} f(s) ds.$$

It is easily seen that if $\gamma = -\alpha$, $\eta = 1$, then

$$D_1^{-\alpha, \alpha} f(t) = t^\alpha {}_a D_t^\alpha f(t).$$

Note that the Caputo modification of the Erdélyi-Kober fractional derivative is also possible [71]. Modeling using Hadamard fractional operator, conformable fractional operator, beta conformable fractional operator and Erdélyi-Kober fractional operator leads to important fractional models. The numerical treatment of these models are essential in related disciplines. The investigation of these topics are beyond the scope of this survey, and we refer interested readers to [61–71] for details

2.2. Mathematical Perspective

We follow the work of Agrawal [58], which investigates **generalized fractional operators** by introducing a **scale function** $z(t)$ and a **weight function** $w(t)$ to the classical Riemann-Liouville or Caputo fractional operators. It is observed that the definitions of Riemann-Liouville and Caputo fractional derivatives depend solely on the fractional inte-

gral and the integer order derivative. Intuitively, one may extend by generalizing them, which is indeed what Agrawal [58] has accomplished.

Generally speaking, Agrawal [58] has generalized fractional integral and integer order derivatives by incorporating a scale function $z(t)$ and a weight function $w(t)$, which gives left/right generalized fractional integral and left/right scaled derivative with respect to $z(t)$ and $w(t)$. To be specific, we have the following definition.

Definition 3. Suppose that $z(t) \in C^1[a, b]$, $z'(t) > 0$, $w(t) \neq 0$. Let $\mathcal{Z}^{-1}(z) : [z(a), z(b)] \rightarrow [a, b]$ with $\mathcal{Z}^{-1}(z(t)) = t$. If $w(\mathcal{Z}^{-1}(z))f(\mathcal{Z}^{-1}(z)) \in L^1(z(a), z(b))$, the **right generalized fractional integral** of function $f(t)$ with respect to $z(t)$ and $w(t)$ is given as follows

$${}_a I_{[z(t); w(t)]}^\alpha f(t) = \frac{[w(t)]^{-1}}{\Gamma(\alpha)} \int_a^t [z(t) - z(s)]^{\alpha-1} [w(s)f(s)] dz(s).$$

Moreover, if $w(t)f(t) \in C^m[a, b]$ and $z(t) \in C^m[a, b]$, then the **left scaled m -th derivative** ($m > 0$ is an integer) of function $f(t)$ with respect to $z(t)$ and $w(t)$ is defined as

$$D_{[z(t); w(t)]}^m f(t) = [w(t)]^{-1} \left(\frac{1}{z'(t)} D_t \right)^m [w(t)f(t)].$$

Remark 1. The extension to $z'(t) < 0$ is trivial. Additionally, as the definitions of left generalized fractional integral and right scaled derivative are not used later, we omit them here.

Using the above two generalized integral and derivative operators, the generalized Riemann-Liouville and generalized Caputo fractional derivatives can be similarly defined as their classical counterparts. Specifically, we have the following definition.

Definition 4. Suppose the conditions in Definition 3 are satisfied. Let $m - 1 < \alpha < m$. For $w(\mathcal{Z}^{-1}(z))f(\mathcal{Z}^{-1}(z)) \in AC^m[z(a), z(b)]$ and $({}_a I_{[z(t); w(t)]}^{m-\alpha})f(t) \in C^m[a, b]$, we have the **generalized left Riemann-Liouville fractional derivative** of order $\alpha > 0$ with respect to the scale function $z(t)$ and weight function $w(t)$, defined as

$${}_a D_{[z(t); w(t)]}^\alpha f(t) = D_{[z(t); w(t)]}^m \left({}_a I_{[z(t); w(t)]}^{m-\alpha} \right) f(t). \quad (1)$$

For $D^m[w(\mathcal{Z}^{-1}(z))f(\mathcal{Z}^{-1}(z))] \in L^1(z(a), z(b))$, the **generalized left Caputo fractional derivative** is defined as

$${}_a^C D_{[z(t); w(t)]}^\alpha f(t) = {}_a I_{[z(t); w(t)]}^{m-\alpha} \left(D_{[z(t); w(t)]}^m f(t) \right). \quad (2)$$

As in Remark 1, the related right operators can be similarly defined and are omitted here; we refer interested readers to [58] for details.

Formulas (1) and (2) are indeed a kind of generalization of fractional derivatives since they will reduce to the classical Riemann-Liouville and classical Caputo fractional derivatives of order α when $z(t) = t$, $w(t) = 1$. It is elucidated in [58] that many equations can be reformulated using this generalized operator and thus can be solved in an unified and elegant way. That is why we need this type of generalized fractional model to unify various fractional models involving different types of fractional derivatives (such as Hadamard, modified Erdélyi-Kober, Riemann-Liouville and Caputo). To better analyze this type of model, some crucial properties of the generalized operator have been developed in [58,59]. Moreover, this generalized operator can be applied to describe anomalous diffusion with a time-dependent diffusivity; see [72] and the related references therein.

So far, we have introduced the generalized fractional operators. Similar to fractional models, models equipped with the generalized fractional operators are called generalized

fractional models. There is no doubt that one may propose other extensions and get different generalized fractional models [73–75]; however, this is out of the scope of this review.

2.3. Application Perspective

The motion of particles or abstract particles is very important in microscopic-level modeling. One of the most powerful tools in microscopic modeling is the stochastic process, and relevant macroscopic equations are used to dig out information from this process. For more information, see [3] and the references therein. In this section, we shall illustrate another generalized fractional model from the relations between the stochastic process and the macroscopic equations that its probability density function satisfies. In what follows, we introduce ideas from [60] and also use similar notations as in [60].

We begin with the Brownian motion B_t . In essence, it is a stochastic process that can be used to describe the motion of pollen particles. It is known that the probability density function of B_t (the probability of particle locates in position x at time t) satisfies standard diffusion equation, i.e.,

$$\partial_t u(x, t) = \Delta u(x, t).$$

If the Brownian motion is time changed by a particular subordinator [76], then it may be typically used to describe anomalous subdiffusion phenomenon. To illustrate this, let S_t be a subordinator (or nondecreasing real-valued Lévy process [17]) with $S_0 = 0$ that is known to be uniquely determined by its Laplace exponent $\phi(\lambda)$ ($E[e^{-\lambda S_t}] = e^{-t\phi(\lambda)}$ for $\lambda > 0$). Denote E_t as its inverse, i.e.,

$$E_t := \inf\{r > 0 : S_r > t\}, \quad t \geq 0.$$

Let us consider the time changed process $Y_t = B_{E_t}$. Suppose that $\phi(\lambda) = \lambda^\alpha$, $\alpha \in (0, 1)$ which implies that S_t is the α -stable subordinator, and B_t is independent of S_t ; then, the probability density function of Y_t is a solution of the typical time fractional equation

$${}_0D_t^\alpha (u(x, t) - u(x, 0)) = \Delta u(x, t).$$

Based on the above discussions, there are two natural extensions of the time changed process Y_t : (i) using a general strong Markov process X_t instead of Brownian motion B_t ; (ii) replacing α -stable subordinator with a general S_t . The first extension will give rise to a more general operator than Δ ; see [60] for details. The second extension will result in a generalization of the Riemann-Liouville fractional operator. To see this, recall that subordinator S_t can be fully characterized by its Laplace exponent $\phi(\lambda)$, which motivates us to achieve S_t by constructing proper $\phi(\lambda)$. With this fact in mind, we consider the following Laplace exponent

$$\phi(\lambda) = \int_0^\infty (1 - e^{-\lambda x}) \mu(dx),$$

where μ is an infinite Lévy measure on $(0, \infty)$ satisfying

$$\int_0^\infty \max\{1, z\} \mu(dz) < \infty,$$

that is assumed to be determined by a right continuous decreasing function $w(t)$ on $(0, \infty)$ (see [60,77] for details). The specific relation is given as $\mu(x, \infty) = w(x)$. Then, it is shown

in [60,77] that this general subordinator will lead to the following generalized fractional operator (the “fractional order” is implicitly given by $w(t)$)

$${}_0D_t^{w(t)}f(t) = \frac{d}{dt} \int_0^t w(t-s)f(s)ds.$$

Obviously, when $w(t) = t^{-\alpha}$, it reduces to the classical Riemann-Liouville fractional derivative. If the phenomenon involves reactions (e.g., chemical reaction), the model will have a reaction term and then the above operator can be further generalized—see [60] for derivations and [4] for its application.

The generalized fractional model with the above generalized fractional operator is naturally derived to understand particular phenomenon [4]. The investigation of this type of model is both interesting and promising.

Until now, we have introduced the origin of (generalized) fractional models from two perspectives. Let us provide some comments on the fractional models vs integer order models. As we discussed before, the fractional model is essentially used to characterize anomalous diffusion processes and other memory processes, while the integer order model is widely used to characterize phenomenon with local nature. Therefore, the choice of model depends closely on the nature of the phenomenon. There are some data-driven situations showing that the fractional model is superior to integer order models. However, these two models are frequently quite close (due to α being close to 1 in some real applications), and it is usual that the fractional model requires much more computation (due to the non-local nature of fractional derivative), as we shall see later in Section 3. In this context, one has to balance the accuracy of the model and the computation cost to make a reasonable choice. There are cases in which the fractional model and the integer order model of a physical system are significantly different (due to α not being close to 1), e.g., energy supply–demand system [10]. In such a case, the accuracy of the model is more important and one may always choose the fractional model instead of integer order model.

In the next section, we shall review some existing numerical methods for (generalized) fractional models.

3. Numerical Methods

In this section, we shall focus on some existing numerical methods of generalized fractional models derived from mathematical perspective and leave the related discussions for models from application perspective for readers (see [78,79]). To be precise, we investigate the following generalized time fractional equation

$$\begin{cases} {}_0^CD_{t;[z(t),1]}^\alpha u(x,t) = \mathcal{L}u(x,t) + f(x,t), & (x,t) \in (a,b) \times (0,T) \\ u(x,0) = \psi(x), & x \in [a,b] \\ u(a,t) = \phi_1(t), \quad u(b,t) = \phi_2(t), & t \in (0,T] \end{cases} \quad (3)$$

where $\phi_1(t)$, $\phi_2(t)$, $\psi(x)$, $f(x,t)$ are given smooth functions, ${}_0^CD_{t;[z(t),1]}^\alpha u(x,t)$ ($0 < \alpha < 1$) is the generalized Caputo fractional derivative with respect to t (see (2)), $z(t)$ satisfies the assumptions in Definition 4, and $\mathcal{L}$ is a linear operator defined as

$$\mathcal{L}u(x,t) = (p(x,t)u_x(x,t))_x - q(x,t)u(x,t),$$

with $p(x,t) \geq p_0 > 0$ and $q(x,t) \geq 0$. The well-posedness of (3) has been addressed in [80–82], and we shall focus on numerical methods from here onwards.

The appearance of the scale function $z(t)$ is used to stretch or contract the time domain. As demonstrated in [58], this may be necessary to accurately capture the phenomenon

of interest over a desired range of time, which could be within micro/nano-seconds, or over several decades. Note that the weight function $w(t) \equiv 1$ in (3). This, however, does not jeopardize the generality of (3) because a similar equation as (3) with a general weight function $w(t)$ can be rewritten to the form (3) by a simple transformation, as observed in [80,81,83–87]. Specifically, if ${}_0^C D_{t;[z(t),1]}^\alpha u(x,t)$ is replaced by ${}_0^C D_{t;[z(t),w(t)]}^\alpha u(x,t)$, then multiplying both sides of the first equation in (3) by $w(t)$ and using the following transformations

$$\tilde{u} = w(t)u(x,t), \quad \tilde{f} = w(t)f(x,t),$$

leads to

$$\begin{cases} {}_0^C D_{t;[z(t),1]}^\alpha \tilde{u}(x,t) = \mathcal{L}\tilde{u}(x,t) + \tilde{f}(x,t), & (x,t) \in (a,b) \times (0,T) \\ \tilde{u}(x,0) = w(0)\psi(x), & x \in [a,b] \\ \tilde{u}(a,t) = w(t)\phi_1(t), \quad \tilde{u}(b,t) = w(t)\phi_2(t), & t \in (0,T) \end{cases}$$

which is exactly the form of (3). We note that a general weight $w(t)$ and $w(t) \equiv 1$ will make a difference if one considers nonlinear problems. Fortunately, we can still apply the proposed method to solve it with u being replaced by wu in the generalized interpolation method, and $u(x, \mathcal{Z}^{-1}(z))$ being replaced by $w(\mathcal{Z}^{-1}(z))u(x, \mathcal{Z}^{-1}(z))$ in the generalized convolution method.

To construct numerical schemes of (3), the two main tasks are discretization of the generalized Caputo fractional derivative and discretization of the linear operator $\mathcal{L}$. The former is the main concern in what follows. For the latter, finite difference [33,35], compact finite difference [33,35,81] or finite element [22] can be applied directly. In this section, we shall first present two types of approximation methods, namely generalized interpolation and generalized convolution quadrature, for the generalized Caputo fractional derivative. This is followed by the approximation of $\mathcal{L}$, and finally we derive the fully discrete numerical schemes of (3). For other methods, one can refer to [88–91] for discontinuous Galerkin method, ref. [92] for the local discontinuous Galerkin method, refs. [93–95] for the spectral method and [22] for the difference type method.

For clarity, we give an explicit expression of ${}_0^C D_{t;[z(t),1]}^\alpha u(x,t)$ ($0 < \alpha < 1$) as

$${}_0^C D_{t;[z(t),1]}^\alpha u(x,t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{1}{[z(t)-z(s)]^\alpha} \frac{\partial u(x,s)}{\partial s} ds. \quad (4)$$

The subsequent approximation methods of the generalized Caputo fractional derivative are based on the expression (4) (see Sections 3.1 and 3.2 below). Let $z(t)$ be a strictly increasing function and

$$P_t : 0 = t_0 < t_1 < \cdots < t_{N-1} < t_N = T,$$

be any partition of $[0, T]$. Corresponding to P_t , we form the partition

$$P_z : z(t_0) = z_0 < z_1 < \cdots < z_{N-1} < z_N = z(t_N).$$

For simplicity, denote $f_n = f(t_n)$, $z_n = z(t_n)$, $u^n(x) = u(x, t_n)$, $\tau_z = (z_N - z_0)/N$ (which will be the step size of P_z if it is a uniform mesh), and

$$\delta_z f_{n+\frac{1}{2}} = \frac{f_{n+1} - f_n}{z_{n+1} - z_n}, \quad \delta_z^2 f_n = \frac{\delta_z f_{n+\frac{1}{2}} - \delta_z f_{n-\frac{1}{2}}}{z_{n+1} - z_{n-1}}.$$

3.1. Generalized Interpolation Method

The main idea of the generalized interpolation method is to apply piecewise generalized Lagrange interpolation to approximate $u(x, t)$. We begin with the generalized Lagrange interpolation. Suppose (z_n, f_n) ($0 \leq n \leq N$) are nodes from $(z(t), f(t))$ on mesh P_t for two given functions $f(t)$ and $z(t)$; then, we have the following definition.

Definition 5 (Generalized Lagrange Interpolation). For $(i + 1)$ consecutive nodes (z_n, f_n) ($k \leq n \leq k + i$), the i -th generalized Lagrange interpolation of these nodes is given by

$$\mathcal{I}_{i,k}^{z(t)} f(t) := \sum_{n=k}^{k+i} \left(\prod_{k \leq j \leq k+i, j \neq n} \frac{z(t) - z_j}{z_n - z_j} \right) f_n. \quad (5)$$

The first order derivative of $\mathcal{I}_{i,k}^{z(t)}(t)$ is frequently used later. In fact, from formula (5), it is easy to obtain

$$\frac{d}{dt} \mathcal{I}_{i,k}^{z(t)}(t) = \sum_{n=k}^{k+i} \sum_{l=k, l \neq n}^{k+i} \frac{\prod_{k \leq j \leq k+i, j \neq n, l} (z(t) - z_j)}{\prod_{i \leq j \leq i+k, j \neq n} (z_n - z_j)} z'(t) f_n. \quad (6)$$

In what follows, we shall present the construction of an approximation method mainly using linear ($i = 1$) and quadratic ($i = 2$) generalized Lagrange interpolation. For convenience, we give an equivalent and simple expression from (6) below,

$$\frac{d\mathcal{I}_{1,k}^{z(t)}(t)}{dt} = \frac{f_{k+1} - f_k}{z_{k+1} - z_k} z'(t) = \left(\delta_z f_{k+\frac{1}{2}} \right) z'(t), \quad (7)$$

$$\frac{d\mathcal{I}_{2,k-1}^{z(t)}(t)}{dt} = \left[\delta_z f_{k+\frac{1}{2}} + \left(\delta_z^2 f_k \right) (2z(t) - z_k - z_{k+1}) \right] z'(t), \quad k \geq 1. \quad (8)$$

Here, we introduce two types of methods depending on whether we discretize (4) at an integer node or non-integer node. For the sake of simplicity, denote $(\gamma \in [0, 1])$

$$\omega_{n,k}^{0,\gamma} = \begin{cases} (z_{n-1+\gamma} - z_k)^{1-\alpha} - (z_{n-1+\gamma} - z_{k+1})^{1-\alpha}, & 0 \leq k \leq n-2 \\ (z_{n-1+\gamma} - z_{n-1})^{1-\alpha}, & k = n-1 \end{cases}$$

$$\omega_{n,k}^{1,\gamma} = 2 \frac{(z_{n-1+\gamma} - z_{k-1})^{2-\alpha} - (z_{n-1+\gamma} - z_k)^{2-\alpha}}{2 - \alpha} - (z_k - z_{k-1}) [(z_{n-1+\gamma} - z_{k-1})^{1-\alpha} + (z_{n-1+\gamma} - z_k)^{1-\alpha}], \quad 1 \leq k \leq n-1.$$

Integer nodes

Now, let us present the approximations of the generalized Caputo fractional derivative (4) using the generalized interpolation method with integer nodes $t = t_n$. Note that (4) can be reformulated in two ways as

$${}_0^C D_{t;[z(t),1]}^\alpha u(x, t_n) = \frac{1}{\Gamma(1-\alpha)} \left[\int_{t_0}^{t_1} [z_n - z(s)]^{-\alpha} \frac{\partial u(x, s)}{\partial s} ds + \sum_{k=1}^{n-1} \int_{t_k}^{t_{k+1}} [z_n - z(s)]^{-\alpha} \frac{\partial u(x, s)}{\partial s} ds \right] \quad (9)$$

$$= \frac{1}{\Gamma(1-\alpha)} \left[\int_{t_0}^{t_2} [z_n - z(s)]^{-\alpha} \frac{\partial u(x, s)}{\partial s} ds + \sum_{k=2}^{n-1} \int_{t_k}^{t_{k+1}} [z_n - z(s)]^{-\alpha} \frac{\partial u(x, s)}{\partial s} ds \right]. \quad (10)$$

3.1.1. gL1 Method

Based on (9), using generalized linear interpolation $\mathcal{I}_{1,k}^{z(t)} u(x, t) \approx u(x, t)$ in $[t_k, t_{k+1}]$ yields the **gL1 method** [82,87,96,97]. To be specific, noting (7) we obtain

$$\begin{aligned} & {}^C_0 D_{t;[z(t),1]}^\alpha u(x, t_n) \\ &= \frac{1}{\Gamma(1-\alpha)} \left[\int_{t_0}^{t_1} [z_n - z(s)]^{-\alpha} \frac{\partial u(x, s)}{\partial s} ds + \sum_{k=1}^{n-1} \int_{t_k}^{t_{k+1}} [z_n - z(s)]^{-\alpha} \frac{\partial u(x, s)}{\partial s} ds \right] \\ &\approx \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{n-1} \int_{t_k}^{t_{k+1}} \frac{1}{[z(t_n) - z(s)]^\alpha} \frac{\partial \mathcal{I}_{1,k}^{z(s)} u(x, s)}{\partial s} ds \\ &= \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{n-1} \int_{t_k}^{t_{k+1}} \frac{1}{[z(t_n) - z(s)]^\alpha} \frac{u^{k+1}(x) - u^k(x)}{z_{k+1} - z_k} z'(s) ds = \frac{1}{\Gamma(2-\alpha)} \sum_{k=0}^{n-1} \omega_{n,k}^{gL1} \delta_z u^{k+\frac{1}{2}}(x), \end{aligned}$$

where the coefficients $\omega_{n,k}^{gL1} = \omega_{n,k}^{0,1}$. In Theorem 1 of [87], the gL1 method is proved to attain $O(\tau_z^{2-\alpha})$ by using the residual of the generalized Lagrange interpolation, i.e.,

$$f(t) - \mathcal{I}_{i,k}^{z(t)} f(t) = \frac{1}{(i+1)!} \left(\frac{d^{i+1}}{dz^{i+1}} g(\xi) \right) \prod_{n=k}^{k+i} (z(t) - z_n), \quad z_k < \xi < z_{k+i}, \quad (11)$$

where $g(z) = f(\mathcal{Z}^{-1}(z))$ and $\mathcal{Z} : t \rightarrow z(t)$ is a strictly increasing mapping function defined over $t \in [0, 1]$. Note that [82,97] consider uniform mesh P_t , and the convergence of the numerical scheme is proven using the Lax-Richtmyer theorem but the order of convergence is not explicitly given, while [87] extends to general mesh and derives the order of convergence.

3.1.2. gL1-2 Method

Based on (9), a high-order **gL1-2 method** [80,96,98] can be derived if one applies generalized linear interpolation $\mathcal{I}_{1,0}^{z(t)} u(x, t) \approx u(x, t)$ in $[t_0, t_1]$ and generalized quadratic interpolation $\mathcal{I}_{2,k-1}^{z(t)} u(x, t) \approx u(x, t)$ in $[t_k, t_{k+1}]$ ($k \geq 1$). Noting (7) and (8), from (9) we obtain

$$\begin{aligned} & {}^C_0 D_{t;[z(t),1]}^\alpha u(x, t_n) \\ &= \frac{1}{\Gamma(1-\alpha)} \left[\int_{t_0}^{t_1} [z_n - z(s)]^{-\alpha} \frac{\partial u(x, s)}{\partial s} ds + \sum_{k=1}^{n-1} \int_{t_k}^{t_{k+1}} [z_n - z(s)]^{-\alpha} \frac{\partial u(x, s)}{\partial s} ds \right] \\ &\approx \frac{1}{\Gamma(1-\alpha)} \left\{ \int_{t_0}^{t_1} \frac{1}{[z_n - z(s)]^\alpha} \frac{\partial \mathcal{I}_{1,0}^{z(s)} u(x, s)}{\partial s} ds + \sum_{k=1}^{n-1} \int_{t_k}^{t_{k+1}} \frac{1}{[z_n - z(s)]^\alpha} \frac{\partial \mathcal{I}_{2,k-1}^{z(s)} u(x, s)}{\partial s} ds \right\} \\ &= \frac{1}{\Gamma(1-\alpha)} \left\{ \sum_{k=0}^{n-1} \delta_z u^{k+\frac{1}{2}}(x) \int_{z_k}^{z_{k+1}} \frac{dz}{[z_n - z]^\alpha} + \sum_{k=1}^{n-1} \delta_z^2 u^k(x) \int_{z_k}^{z_{k+1}} \frac{2z - z_k - z_{k+1}}{[z_n - z]^\alpha} dz \right\} \\ &= \frac{1}{\Gamma(2-\alpha)} \left[\sum_{k=0}^{n-1} \omega_{n,k}^0 \delta_z u^{k+\frac{1}{2}}(x) + \sum_{k=1}^{n-1} \omega_{n,k}^1 \delta_z^2 u^k(x) \right] = \frac{1}{\Gamma(2-\alpha)} \sum_{k=0}^{n-1} \omega_{n,k}^{gL1-2} \delta_z u^{k+\frac{1}{2}}(x), \end{aligned}$$

where $\omega_{n,k}^{gL1-2} = \omega_{n,0}^{0,1}$ when $n = 1$, and for $n \geq 2$ we have

$$\omega_{n,k}^{gL1-2} = \begin{cases} \omega_{n,0}^{0,1} - \bar{\omega}_{n,1}^{1,1}, & k = 0 \\ \omega_{n,k}^{0,1} + \bar{\omega}_{n,k}^{1,1} - \bar{\omega}_{n,k+1}^{1,1}, & 1 \leq k \leq n-2 \\ \omega_{n,n-1}^{0,1} + \bar{\omega}_{n,n-1}^{1,1}, & k = n-1 \end{cases}$$

with $\bar{\omega}_{n,k}^{1,1} = \frac{\omega_{n,k}^{1,1}}{z_{k+1} - z_{k-1}}$, $k \geq 1$. Similarly, using the residual of the generalized Lagrange interpolation, it is shown that the gL1-2 method achieves $O(\tau_z^{3-\alpha})$ for general mesh (see Theorem 3.1 in [80]), but the analysis of the resulting fully discrete scheme to solve the generalized time fractional problem (3) is not easy; see Section 3.4 later. In fact, [80] only proves the convergence for a small range of α using the energy method, while the proof for all α is given in [96,98] by analyzing the coefficient matrix directly, which requires very careful analysis of coefficients. Possibly, one can extend a different L1-2 proposed in [37,39,40] for uniform or graded mesh using generalized interpolations, and provide an easier solution.

3.1.3. gL2 Method

Alternatively, based on the representation (10), a different L2 type method, namely the **gL2 method**, can be constructed using only generalized quadratic interpolation, i.e., $\mathcal{I}_{2,0}^{z(t)} u(x, t) \approx u(x, t)$ in $[t_0, t_2]$ and $\mathcal{I}_{2,k-1}^{z(t)} u(x, t) \approx u(x, t)$ in $[t_k, t_{k+1}]$ ($k \geq 2$). Similar to the above derivation procedure, from (10) it is found that

$$\begin{aligned} & {}_0^C D_{t;[z(t),1]}^\alpha u(x, t_n) \\ &= \frac{1}{\Gamma(1-\alpha)} \left[\int_{t_0}^{t_2} [z_n - z(s)]^{-\alpha} \frac{\partial u(x, s)}{\partial s} ds + \sum_{k=2}^{n-1} \int_{t_k}^{t_{k+1}} [z_n - z(s)]^{-\alpha} \frac{\partial u(x, s)}{\partial s} ds \right] \\ &\approx \frac{1}{\Gamma(1-\alpha)} \left\{ \int_{t_0}^{t_2} \frac{\partial \mathcal{I}_{2,0}^{z(s)} u(x, s)}{\partial s} \frac{ds}{[z(t_n) - z(s)]^\alpha} + \sum_{k=2}^{n-1} \int_{t_k}^{t_{k+1}} \frac{\partial \mathcal{I}_{2,k-1}^{z(s)} u(x, s)}{\partial s} \frac{ds}{[z(t_n) - z(s)]^\alpha} \right\} \\ &= \frac{1}{\Gamma(1-\alpha)} \int_{t_0}^{t_2} \left[\delta_z^2 u^1(x) (2z(s) - z_2 - z_1) + \delta_z u^{\frac{3}{2}}(x) \right] \frac{dz(s)}{[z(t_n) - z(s)]^\alpha} \\ &\quad + \frac{1}{\Gamma(1-\alpha)} \sum_{k=2}^{n-1} \int_{t_k}^{t_{k+1}} \left[\delta_z^2 u^k(x) (2z(t) - z_{k+1} - z_k) + \delta_z u^{k+\frac{1}{2}}(x) \right] \frac{dz(s)}{[z(t_n) - z(s)]^\alpha} \\ &= \frac{1}{\Gamma(2-\alpha)} \sum_{k=0}^{n-1} \omega_{n,k}^{gL2} \delta_z u^{k+\frac{1}{2}}(x), \end{aligned}$$

where $\omega_{n,k}^{gL2}$ is given as follows:

- when $n = 2$,

$$\omega_{n,k}^{gL2} = \begin{cases} \omega_{n,0}^{0,1} - \frac{2r_1}{1+r_1} \frac{\omega_{n,0}^{1,1}}{z_1 - z_0} - \frac{2}{1+r_1} \frac{\omega_{n,1}^{1,1}}{z_2 - z_1}, & k = 0 \\ \omega_{n,1}^{0,1} + \frac{2r_1}{1+r_1} \frac{\omega_{n,0}^{1,1}}{z_1 - z_0} + \frac{2}{1+r_1} \frac{\omega_{n,1}^{1,1}}{z_2 - z_1}, & k = 1 \end{cases}$$

- when $n \geq 3$,

$$\omega_{n,k}^{gL2} = \begin{cases} \omega_{n,0}^{0,1} - \frac{2r_1}{1+r_1} \frac{\omega_{n,0}^{1,1}}{z_1 - z_0} - \frac{2}{1+r_1} \frac{\omega_{n,1}^{1,1}}{z_2 - z_1}, & k = 0 \\ \omega_{n,1}^{0,1} + \frac{2r_1}{1+r_1} \frac{\omega_{n,0}^{1,1}}{z_1 - z_0} + \frac{2}{1+r_1} \frac{\omega_{n,1}^{1,1}}{z_2 - z_1} - \frac{2}{1+r_2} \frac{\omega_{n,2}^{1,1}}{z_3 - z_2}, & k = 1 \\ \omega_{n,k}^{0,1} + \frac{2}{1+r_k} \frac{\omega_{n,k}^{1,1}}{z_{k+1} - z_k} - \frac{2}{1+r_{k+1}} \frac{\omega_{n,k-1}^{1,1}}{z_k - z_{k-1}}, & 2 \leq k \leq n-2 \\ \omega_{n,n-1}^{0,1} + \frac{2}{1+r_{n-1}} \frac{\omega_{n,n-1}^{1,1}}{z_n - z_{n-1}}, & k = n-1 \end{cases}$$

with $r_k = \frac{z_k - z_{k-1}}{z_{k+1} - z_k}$. To analyze the accuracy of the gL2 method, the main tool is still the residual of the generalized Lagrange interpolation, though the analysis is more technical (see Lemma 2.1 and Theorem 2.1 in [81]). Indeed, this method gives the same order of accuracy $3 - \alpha$ as the gL1-2 method, and the convergence analysis for the resulting fully discrete scheme to solve the generalized time fractional problem (3) can be conducted for all α ; see [35,81] for details. One drawback of this gL2 method-based fully discrete scheme is that one needs other low-order methods to compute $u(x, t_1)$. Fortunately, the convergence order can be kept if a reasonable smaller step size is taken in $[t_0, t_1]$. Alternatively, one can tackle it using the Hermite interpolation method proposed in [41].

Non-integer nodes

We shall now approximate the generalized Caputo fractional derivative (4) using generalized interpolation method with non-integer nodes $t = t_{n-1+\sigma}$, where $\sigma = 1 - \frac{\alpha}{2}$. From (4), we can write

$${}_0^C D_{t;[z(t),1]}^\alpha u(x, t_{n-1+\sigma}) = \frac{1}{\Gamma(1-\alpha)} \left[\sum_{k=0}^{n-2} \int_{t_k}^{t_{k+1}} [z_{n-1+\sigma} - z(s)]^{-\alpha} \frac{\partial u(x, s)}{\partial s} ds + \int_{t_{n-1}}^{t_{n-1+\sigma}} [z_{n-1+\sigma} - z(s)]^{-\alpha} \frac{\partial u(x, s)}{\partial s} ds \right], \quad (12)$$

where $z_{n-1+\sigma} = (1 - \sigma)z_{n-1} + \sigma z_n$ and $t_{n-1+\sigma} = \mathcal{Z}^{-1}(z_{n-1+\sigma})$.

3.1.4. gL2-1 $_\sigma$ Method

In (12), we apply generalized quadratic interpolation $\mathcal{I}_{2,k}^{z(t)} u(x, t) \approx u(x, t)$ in $[t_k, t_{k+1}]$ ($0 \leq k \leq n-2$) and generalized linear interpolation $\mathcal{I}_{1,n-1}^{z(t)} u(x, t) \approx u(x, t)$ in $[t_{n-1}, t_{n-1+\sigma}]$, leading to the **gL2-1 $_\sigma$ method**, also known as the **generalized Alikhanov's method** [35,86]. Specifically, we find

$$\begin{aligned} & {}_0^C D_{t;[z(t),1]}^\alpha u(x, t_{n-1+\sigma}) \\ &= \frac{1}{\Gamma(1-\alpha)} \left[\sum_{k=0}^{n-2} \int_{t_k}^{t_{k+1}} + \int_{t_{n-1}}^{t_{n-1+\sigma}} \right] [z_{n-1+\sigma} - z(s)]^{-\alpha} \frac{\partial u(x, s)}{\partial s} ds \\ &\approx \frac{1}{\Gamma(1-\alpha)} \left\{ \sum_{k=0}^{n-2} \int_{t_k}^{t_{k+1}} \frac{\partial \mathcal{I}_{2,k}^{z(s)} u(x, s)}{\partial s} \frac{ds}{[z_{n-1+\sigma} - z(s)]^\alpha} + \int_{t_{n-1}}^{t_{n-1+\sigma}} \frac{\partial \mathcal{I}_{1,n-1}^{z(s)} u(x, s)}{\partial s} \frac{ds}{[z_{n-1+\sigma} - z(s)]^\alpha} \right\} \\ &= \frac{1}{\Gamma(1-\alpha)} \left\{ \sum_{k=0}^{n-2} \int_{t_k}^{t_{k+1}} \frac{\delta_z u^{k+\frac{1}{2}}(x) dz(s)}{[z_{n-1+\sigma} - z(s)]^\alpha} + \int_{t_{n-1}}^{t_{n-1+\sigma}} \frac{\delta_z u^{n-\frac{1}{2}}(x) dz(s)}{[z_{n-1+\sigma} - z(s)]^\alpha} \right\} \\ &\quad + \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{n-2} \delta_z^2 u^{k+1}(x) \int_{t_k}^{t_{k+1}} \frac{2z(s) - z_k - z_{k+1}}{[z_{n-1+\sigma} - z(s)]^\alpha} dz(s) \\ &= \frac{1}{\Gamma(2-\alpha)} \left[\sum_{k=0}^{n-1} \omega_{n,k}^{0,\sigma} \delta_z u^{k+\frac{1}{2}}(x) + \sum_{k=1}^{n-1} \omega_{n,k}^{1,\sigma} \delta_z^2 u^k(x) \right] = \frac{1}{\Gamma(2-\alpha)} \sum_{k=0}^{n-1} \omega_{n,k}^{gL2-1_\sigma} \delta_z u^{k+\frac{1}{2}}(x), \end{aligned}$$

where $\omega_{n,0}^{gL2-1_\sigma} = \omega_{n,0}^{0,\sigma}$ when $n = 1$, and for $n \geq 2$ we have

$$\omega_{n,k}^{gL2-1_\sigma} = \begin{cases} \omega_{n,0}^{0,\sigma} - \bar{\omega}_{n,0}^{1,\sigma}, & k = 0 \\ \omega_{n,k}^{0,\sigma} + \bar{\omega}_{n,k}^{1,\sigma} - \bar{\omega}_{n,k+1}^{1,\sigma}, & 1 \leq k \leq n-2 \\ \omega_{n,n-1}^{0,\sigma} + \bar{\omega}_{n,n-1}^{1,\sigma}, & k = n-1 \end{cases}$$

where $\bar{\omega}_{n,k}^{1,\sigma} = \frac{\omega_{n,k}^{1,\sigma}}{z_{k+1} - z_{k-1}}$, $k \geq 1$. It is proved in [80] (see Theorem 3.2) that the above derived approximation gives $O(\tau_z^{3-\alpha})$. Moreover, it is shown in [35] that this method can also be used to solve variable order ($\alpha = \alpha(x, t)$) problems. Though the gL2-1 $_{\sigma}$ method gives as good approximation properties as previous high-order methods, we can only obtain $O(\tau_z^2)$ for the fully discrete numerical scheme for solving (3) because

$$\mathcal{L}u(x, t_{n-1+\sigma}) = (1 - \sigma)\mathcal{L}u(x, t_{n-1}) + \sigma\mathcal{L}u(x, t_n) + \sigma(1 - \sigma)O(\tau_z^2), \quad (13)$$

is adopted in the numerical scheme construction.

To summarize Section 3.1, the generalized interpolation based approximation methods can be written in a **unified form** as follows.

Theorem 1. Assume that $u(\cdot, \mathcal{Z}^{-1}(z)) \in C^r[z(0), z(T)]$, where $r = 2$ for gL1 and $r = 3$ for gL1-2, gL2, gL2-1 $_{\sigma}$. We have

$${}_0^C D_{t;[z(t),1]}^{\alpha} u(x, t_{n-1+\gamma}) = \frac{1}{\Gamma(2-\alpha)} \sum_{k=0}^{n-1} \omega_{n,k}^* \delta_z u^{k+\frac{1}{2}}(x) + O(\tau_z^{\beta}), \quad (14)$$

where $\gamma = 1$ for gL1, gL1-2, gL2 and $\gamma = \sigma$ for gL2-1 $_{\sigma}$, * denotes the type of method (gL1, gL1-2, gL2 or gL2-1 $_{\sigma}$), and β is the corresponding order of accuracy with $\beta = 2 - \alpha$ for gL1 and $\beta = 3 - \alpha$ for gL1-2, gL2, gL2-1 $_{\sigma}$.

Proof. Combining the technique of integration by parts with a residual of generalized interpolation (11), one can derive the approximation errors. For details, see [87] for the gL1 method, ref. [86] for the gL2-1 $_{\sigma}$ method, ref. [80] for the gL1-2 and gL2-1 $_{\sigma}$ methods, and [81] for the gL2 method. $\square$

Remark 2. Based on the above discussions, β can be $3 - \alpha$ or higher for general mesh (see [99] for the construction using high-order generalized interpolations). However, the analysis of the resulting fully discrete scheme for solving (3) is challenging; see Section 3.4 later.

Remark 3. As far as we know, the best accuracy of the generalized interpolation method-based fully discrete scheme is $O(\tau_z^{3-\alpha})$ for uniform z mesh, and $O(N^{-(2-\alpha)})$ for general mesh. Hopefully, by making subtle changes and applying correction techniques when necessary, it is possible to provide a rigorous analysis of high-order generalized interpolation-based methods for general mesh; see [37,39,100] and the references therein.

Remark 4. The approximation error in (14) holds with high regularity assumption of u . If the assumption is violated, (14) does not hold any more and the worst case is that all methods degenerate to $O(\tau_z)$. A mature technique to recover the accuracy is to apply graded mesh [27,37], quasi-graded mesh [30] or more general mesh [31,36,40,44]. The investigation of this technique is out of the scope of this work and we refer interested readers to the related references.

3.2. Generalized Convolution Quadrature Method

Let us briefly introduce the classical convolution quadrature method [23,25,45] that aims to approximate the Riemann-Liouville fractional derivative ${}_0 D_t^{\alpha} f(t)$ (see Section 2.1 of this work and also [1,2]) with uniform mesh accurately. Here, we consider $0 < \alpha < 1$ and denote $\tau = \frac{T}{N}$ as the step size of the uniform mesh $P_t : 0 = t_0 < t_1 < \dots < t_{N-1} < t_N = T$. The convolution quadrature approximation is formulated as

$${}_0 D_t^{\alpha} f(t) = \tau^{-\alpha} \sum_{n=0}^{\infty} q_{n,k}^{\alpha} f(t - n\tau) + O(\tau^k),$$

where $q_{n,k}^\alpha$ is the coefficient computed from the generating function of the fractional linear multistep method, that is,

$$\delta_\alpha(\xi) = \left(\sum_{i=1}^k \frac{(1-\xi)^i}{i} \right)^\alpha = \sum_{n=0}^{\infty} q_{n,k}^\alpha \xi^n.$$

Note that when $\alpha = 1$, it reduces to the standard BDFk method [49], and when $k = 1$, it becomes the classical Grünwald-Letnikov (GL) method [1]. The above convolution quadrature method is the starting point to achieve a high-order accuracy method either by using a correction technique for $k \geq 2$, or by assembling a shifted low-order method ($k = 1$).

The **generalized convolution quadrature method** is actually an extension of the above method so that it can be used to approximate (4) efficiently. It depends on the two relations below.

1. The relation between generalized Riemann-Liouville fractional operator and generalized Caputo fractional operator when $f(0) = 0$ (see Theorem 2.2 in [85]), given as

$${}_0^C D_{t;[z(t),1]}^\alpha f(t) = {}_0 D_{t;[z(t),1]}^\alpha f(t), \quad \alpha \in (0,1).$$

2. The relation between generalized Riemann-Liouville fractional operator and classical Riemann-Liouville fractional operator (see (2.12) in [85]),

$${}_0 D_{t;[z(t),1]}^\alpha f(t) = {}_{z_0} D_z^\alpha \bar{f}(z),$$

where $\bar{f}(z) = f(\mathcal{Z}^{-1}(z))$.

From these two relations, it is found that we may construct approximations of (4) by using existing approximation methods of classical Riemann-Liouville fractional derivative, i.e., ${}_{z_0} D_z^\alpha \bar{f}(z)$. Moreover, we need uniform z mesh which is vital in the construction. Fortunately, this uniform z mesh can be achieved by selecting appropriate mesh P_t , such that

$$P_z : z(t_0) = z_0 < z_1 < \cdots < z_{N-1} < z_N = z(t_N),$$

is uniform. Based on the above discussions, the generalized convolution quadrature method of (4) can be constructed by first applying the classical convolution quadrature method for ${}_{z_0} D_z^\alpha \bar{f}(z)$ based on uniform z mesh P_z and then transforming the variable z into variable t using $\mathcal{Z}(t) = z(t)$. In this sense, we are able to obtain $O(\tau_z^k)$ for the generalized BDFk method.

In practice, we take $k = 1$, which results in the generalized Grünwald-Letnikov (gGL) method [83–85], that is,

$${}_0^C D_{t;[z(t),1]}^\alpha f(t_n) = \tau_z^{-\alpha} \sum_{i=0}^n q_{i,1}^\alpha f^{n-i} + O(\tau_z),$$

where $q_{0,1}^\alpha = 1$ and $q_{i,1}^\alpha = (1 - \frac{\alpha+1}{i})q_{i-1,1}^\alpha$ for $i \geq 1$. Then, we consider the linear combinations of shifted gGL methods to obtain high-order accuracy. For this purpose, define the **shifted gGL operator** as follows.

Definition 6 (Shifted gGL operator). Given an integer shift p and a sequence $\{f^i\}$, the corresponding shifted generalized Grünwald-Letnikov operator gGL_p^α is given as

$$gGL_p^\alpha f^n = \tau_z^{-\alpha} \sum_{i=0}^{n+p} q_{i,1}^\alpha f^{n-i+p}.$$

3.2.1. gWSGL with Two Shifts

Similarly to the weighted shifted Grünwald-Letnikov (WSGL) method [56] that is a linear combination of shifted GL methods, we have constructed the **generalized weighted shifted Grünwald-Letnikov (gWSGL) method with two shifts** [85]. To be specific, for the generalized Caputo fractional derivative (4), we obtain (see Theorem 2.1 in [85] for details)

$$\begin{aligned} {}_0^C D_{t;[z(t),1]}^\alpha u(x, t_n) &= \frac{\alpha - 2p_2}{2(p_1 - p_2)} gGL_{p_1}^\alpha u^n(x) + \frac{2p_1 - \alpha}{2(p_1 - p_2)} gGL_{p_2}^\alpha u^n(x) + O(\tau_z^2) \\ &= \tau_z^{-\alpha} \sum_{i=0}^n \lambda_{i,\alpha,2} u^{n-i}(x) + O(\tau_z^2), \end{aligned} \quad (15)$$

where for $p_1 = 1$ and $p_2 = -1$

$$\lambda_{0,\alpha,2} = \frac{\alpha + 2}{2}, \quad \lambda_{i,\alpha,2} = \frac{\alpha + 2}{2} q_{i,1}^\alpha - \frac{\alpha}{2} q_{i-1,1}^\alpha, \quad i \geq 1.$$

3.2.2. gWSGL with Three Shifts

It is possible to apply more shifts to obtain high-order methods. If we apply **three shifts** (see Theorem 2.1 in [83]), then it is found that

$$\begin{aligned} {}_0^C D_{t;[z(t),1]}^\alpha u(x, t_n) &= \rho_{2,1} gGL_{p_1}^\alpha u^n(x) + \rho_{2,2} gGL_{p_2}^\alpha u^n(x) + \rho_{2,3} gGL_{p_3}^\alpha u^n(x) + O(\tau_z^3) \\ &= \tau_z^{-\alpha} \sum_{i=0}^n \lambda_{i,\alpha,3} u^{n-i}(x) + O(\tau_z^3), \end{aligned} \quad (16)$$

where

$$\begin{aligned} \rho_{2,1} &= \frac{12p_2p_3 - (6p_2 + 6p_3 + 1)\alpha + 3\alpha^2}{12(p_1 - p_2)(p_1 - p_3)}, \\ \rho_{2,2} &= \frac{12p_1p_3 - (6p_1 + 6p_3 + 1)\alpha + 3\alpha^2}{12(p_2 - p_1)(p_2 - p_3)}, \\ \rho_{2,3} &= \frac{12p_1p_2 - (6p_1 + 6p_2 + 1)\alpha + 3\alpha^2}{12(p_3 - p_1)(p_3 - p_2)}, \end{aligned}$$

and if $p_1 = 0, p_2 = -1, p_3 = -2$, then

$$\lambda_{0,\alpha,3} = \rho_{2,1} q_{0,1}^\alpha, \quad \lambda_{1,\alpha,3} = \rho_{2,1} q_{1,1}^\alpha + \rho_{2,2} q_{0,1}^\alpha, \quad \lambda_{i,\alpha,3} = \rho_{2,1} q_{i,1}^\alpha + \rho_{2,2} q_{i-1,1}^\alpha + \rho_{2,3} q_{i-2,1}^\alpha, \quad i \geq 2.$$

3.2.3. gWSGL with Four Shifts

In [84], **four shifts** have been employed. The final high-order approximation (see Theorem 2.1 in [84]) with shifts 0, −1, −2, −3 is given as

$$\begin{aligned} {}_0^C D_{t;[z(t),1]}^\alpha u(x, t_n) &= \rho_{3,1} gGL_0^\alpha u^n(x) + \rho_{3,2} gGL_{-1}^\alpha u^n(x) + \rho_{3,3} gGL_{-2}^\alpha u^n(x) + \rho_{3,4} gGL_{-3}^\alpha u^n(x) + O(\tau_z^4) \\ &= \tau_z^{-\alpha} \sum_{i=0}^n \lambda_{i,\alpha,4} u^{n-i}(x) + O(\tau_z^4), \end{aligned} \quad (17)$$

where

$$\begin{aligned}\rho_{3,1} &= \frac{\alpha^3 + 11\alpha^2 + 40\alpha + 48}{48}, & \rho_{3,2} &= \frac{-3\alpha^3 - 27\alpha^2 - 62\alpha}{48}, \\ \rho_{3,3} &= \frac{3\alpha^3 + 21\alpha^2 + 28\alpha}{48}, & \rho_{3,4} &= \frac{-\alpha^3 - 5\alpha^2 - 6\alpha}{48},\end{aligned}$$

and

$$\begin{aligned}\lambda_{0,\alpha,4} &= \rho_{3,1}q_{0,1}^\alpha, & \lambda_{2,\alpha,4} &= \rho_{3,1}q_{2,1}^\alpha + \rho_{3,2}q_{1,1}^\alpha + \rho_{3,3}q_{0,1}^\alpha, \\ \lambda_{1,\alpha,4} &= \rho_{3,1}q_{1,1}^\alpha + \rho_{3,2}q_{0,1}^\alpha, & \lambda_{i,\alpha,4} &= \rho_{3,1}q_{i,1}^\alpha + \rho_{3,2}q_{i-1,1}^\alpha + \rho_{3,3}q_{i-2,1}^\alpha + \rho_{3,4}q_{i-3,1}^\alpha, \quad i \geq 3.\end{aligned}$$

In applications, one can apply gWSGL with two shifts (15) [85] to solve (3) directly. For gWSGL with three and four shifts, namely (16) and (17) [83,84], the solution at $t = t_1$ or/and $t = t_2$ is required to start the fully discrete scheme. This can be performed by using Hermite interpolation and generalized Riemann-Liouville fractional integral; see [83,84] for details. Intuitively, we may take large k (≥ 2) to obtain high-order methods directly (see [25]) and then consider linear combinations of its shifted version to obtain even higher order methods (see [14,57]).

To summarize, in Section 3.2 we present the main idea of the generalized convolution quadrature method and derived various gWSGL methods based on shifted generalized convolution quadrature with $k = 1$ (or equivalently shifted gGL), and discussed its usage in practice. From (15)–(17), it is obvious that they have similar formulations and thus can be written in a **unified form**. Specifically, we have the following.

Theorem 2. If $u(\cdot, \mathcal{L}^{-1}(z)) \in C^{2+s}[z(0), z(T)]$, $s = 2, 3, 4$ and $\frac{d^i}{dz^i}u(\cdot, z(0)) = 0$, $0 \leq i \leq s + 2$, then

$${}_0^C D_{t;[z(t),1]}^\alpha u(x, t_n) = \tau_z^{-\alpha} \sum_{i=0}^n \lambda_{i,\alpha,s} u^{n-i}(x) + O(\tau_z^s), \quad (18)$$

where $s = 2, 3, 4$ denotes two, three and four shifts, respectively.

Proof. The proof of the above results mainly relies on the Fourier transform techniques; see [85] for $s = 2$, [84] for $s = 3$, and [83] for $s = 4$. $\square$

Remark 5. The weights in (18) are exactly the same as in the classical methods but the nodes with respect to the variable t are no longer uniform. In fact, the nodes t_n are carefully chosen such that $P_z = \{z(t_n)\}$ is uniformly distributed.

Remark 6. If we employ the classical interpolation method on nodes t_n that yield a uniform P_z , we shall obtain the same result as gL1 [87] or gL2 [81,86] type methods derived by the generalized interpolation technique.

Remark 7. The order reduction is also observed as in Remark 4. One may apply the correction technique in [22] to recover the accuracy.

3.3. Approximation of $\mathcal{L}$

To derive the fully discrete scheme for the generalized time fractional Equation (3), one can approximate the generalized Caputo fractional derivative (discussed in Sections 3.1 and 3.2), as well as approximate the operator $\mathcal{L}$. As stated at the beginning, we only introduce finite difference and compact finite difference methods for $\mathcal{L}$ and leave other methods to the readers. Here, we follow the works in [33,35,81,101] and present the results directly.

Let P_x be a uniform partition of $[a, b]$, i.e.,

$$P_x : a = x_0 < x_1 < \cdots < x_{M-1} < x_M = b,$$

and denote $h = \frac{b-a}{M}$, $u_j^n = u(x_j, t_n)$, $u_{j+\frac{1}{2}}^n = u(x_{j+\frac{1}{2}}, t_n)$ and $\delta_x u_{j+\frac{1}{2}}^n = \frac{u_{j+1}^n - u_j^n}{x_{j+1} - x_j}$.

3.3.1. Finite Difference Method for $\mathcal{L}$

Considering the discretization at node (x_j, t_n) , the **finite difference approximation** of $\mathcal{L}$ (see Lemma 5 in [33] and Lemma 3.1 in [35]) is given by

$$\begin{aligned}\mathcal{L}u(x_j, t_n) &= \frac{p_{j+\frac{1}{2}}^n u_{j+1}^n - (p_{j+\frac{1}{2}}^n + p_{j-\frac{1}{2}}^n) u_j^n + p_{j-\frac{1}{2}}^n u_{j-1}^n}{h^2} - q_j^n u_j^n + O(h^2) \\ &= \frac{1}{h} \left(p_{j+\frac{1}{2}}^n \delta_x u_{j+\frac{1}{2}}^n - p_{j-\frac{1}{2}}^n \delta_x u_{j-\frac{1}{2}}^n \right) - q_j^n u_j^n + O(h^2).\end{aligned}\quad (19)$$

Obviously, it gives second-order accuracy in the spatial dimension for $u(x, \cdot) \in C^4[a, b]$ and smooth p, q .

3.3.2. Compact Finite Difference Method for $\mathcal{L}$

For compact finite difference approximation of $\mathcal{L}$, we need the following **time-dependent compact finite difference (TDCFD) operator** [81].

Definition 7 (TDCFD operator). Let $d(x, t) = \frac{p_x(x, t)}{p(x, t)}$. For a given function $v(x, t)$, the time-dependent compact finite difference operator H is defined as

$$Hv_j^n = v_j^n + \frac{h^2}{12} \left(\frac{v_{j+1}^n - 2v_j^n + v_{j-1}^n}{h^2} - \frac{d_{j+1}^n v_{j+1}^n - d_{j-1}^n v_{j-1}^n}{2h} \right), \quad 1 \leq j \leq M-1.$$

Applying the TDCFD operator H to $\mathcal{L}u(x_j, t_n)$ and noting the definition of the operator $\mathcal{L}$, we have

$$H\mathcal{L}u(x_j, t_n) = H \underbrace{\partial_x(p(x, t) \partial_x u(x, t))}_{:=v_j^n} \big|_{x=x_j, t=t_n} - Hq_j^n u_j^n.$$

From [81,101], for smooth p and $u(x, \cdot) \in C^6[a, b]$, we obtain

$$Hv_j^n = \frac{1}{h} \left(\psi_{j+\frac{1}{2}}^n \delta_x u_{j+\frac{1}{2}}^n - \psi_{j-\frac{1}{2}}^n \delta_x u_{j-\frac{1}{2}}^n \right) + O(h^4),$$

where

$$\psi(x, t) = p(x, t) - \frac{h^2}{12} \left[\frac{(p_x(x, t))^2}{p(x, t)} - \frac{p_{xx}(x, t)}{2} \right].$$

Hence, the **compact finite difference approximation** of $\mathcal{L}$ is constructed as

$$H\mathcal{L}u(x_j, t_n) = \frac{1}{h} \left(\psi_{j+\frac{1}{2}}^n \delta_x u_{j+\frac{1}{2}}^n - \psi_{j-\frac{1}{2}}^n \delta_x u_{j-\frac{1}{2}}^n \right) - Hq_j^n u_j^n + O(h^4), \quad (20)$$

which achieves fourth-order accuracy in the spatial dimension. Note that [33,35] also considers the compact finite difference method for the special case $p(x, t) = p(t)$, i.e., the function p is independent of x . The dependence of the function p on x will bring difficulties in proving the convergence of the fully discrete scheme of (3) and thus new analysis techniques [81] are required here.

3.4. Fully Discrete Scheme

The fully discrete scheme of (3) can be readily derived using the approximation of $\mathcal{L}$ discussed in Section 3.3, coupled with the approximation of ${}_0^C D_{t;[z(t), 1]}^\alpha u(x, t)$ discussed in Sections 3.1 and 3.2. To show the derivation of the fully discrete scheme, as an example, we shall take the **generalized interpolation method** (Section 3.1) and combine it with finite

difference and compact finite difference methods, respectively. The fully discrete schemes utilizing the generalized convolution quadrature method (Section 3.2) can be similarly derived, and we omit it here.

3.4.1. Finite Difference (FD) Method

We begin with the construction of the fully discrete scheme based on the finite difference (FD) method. Consider the discretization of (3) at the point $(x_j, t_{n-1+\gamma})$, where $\gamma = 1$ or σ ($\sigma = 1 - \frac{\alpha}{2}$). It is obvious from (3) and (13) that

$$\begin{aligned} {}^C_0 D_{t;[z(t),1]}^\alpha u(x_j, t_{n-1+\gamma}) &= \mathcal{L}u(x_j, t_{n-1+\gamma}) + f(x_j, t_{n-1+\gamma}) \\ &= (1-\gamma)\mathcal{L}u(x_j, t_{n-1}) + \gamma\mathcal{L}u(x_j, t_n) + f_j^{n-1+\gamma} + \gamma(1-\gamma)O(\tau_z^2). \end{aligned}$$

Applying the finite difference approximation (19) of $\mathcal{L}$ and the generalized interpolation method (14) for ${}^C_0 D_{t;[z(t),1]}^\alpha u(x_j, t_{n-1+\gamma})$, we obtain

$$\begin{aligned} &\frac{1}{\Gamma(2-\alpha)} \sum_{k=0}^{n-1} \omega_{n,k}^* \delta_z u^{k+\frac{1}{2}}(x_j) + O(\tau_z^\beta) \\ &= (1-\gamma) \left[\frac{p_{j+\frac{1}{2}}^{n-1} \delta_x u_{j+\frac{1}{2}}^{n-1} - p_{j-\frac{1}{2}}^{n-1} \delta_x u_{j-\frac{1}{2}}^{n-1}}{h} - q_j^{n-1} u_j^{n-1} \right] + \gamma \left[\frac{p_{j+\frac{1}{2}}^n \delta_x u_{j+\frac{1}{2}}^n - p_{j-\frac{1}{2}}^n \delta_x u_{j-\frac{1}{2}}^n}{h} - q_j^n u_j^n \right] \\ &\quad + f_j^{n-1+\gamma} + \gamma(1-\gamma)O(\tau_z^2) + O(h^2). \end{aligned}$$

From the above formula, it is readily seen that even if $\beta > 2$ (for example, when $\beta = 3 - \alpha$), the resulting method can only achieve $O(\tau_z^2)$ for $\gamma = \sigma$. After omitting small terms, the fully discrete scheme of (3) based on finite difference method is obtained as follows

$$\begin{aligned} \frac{1}{\Gamma(2-\alpha)} \sum_{k=0}^{n-1} \omega_{n,k}^* \delta_z u^{k+\frac{1}{2}}(x_j) &= (1-\gamma) \left[\frac{p_{j+\frac{1}{2}}^{n-1} \delta_x u_{j+\frac{1}{2}}^{n-1} - p_{j-\frac{1}{2}}^{n-1} \delta_x u_{j-\frac{1}{2}}^{n-1}}{h} - q_j^{n-1} u_j^{n-1} \right] \\ &\quad + \gamma \left[\frac{p_{j+\frac{1}{2}}^n \delta_x u_{j+\frac{1}{2}}^n - p_{j-\frac{1}{2}}^n \delta_x u_{j-\frac{1}{2}}^n}{h} - q_j^n u_j^n \right] + f_j^{n-1+\gamma}, \quad (21) \end{aligned}$$

which can be solved numerically with appropriate initial condition $u_j^0 = \psi(x_j)$ and boundary conditions $u_0^n = \phi_1(t_n)$, $u_M^n = \phi_2(t_n)$.

Applying techniques from (Theorems 2 and 3, [87]), (Theorems 3.1–3.3, [81]) and (Theorems 4.1–4.3, [86]), we can prove the following stability and convergence results for gL1, gL2 and gL2-1 $_\sigma$ methods.

Theorem 3 (Stability of FD-based scheme (21; see [81,86,87])). *If P_z is uniformly distributed, then the numerical scheme (21) is robust (or stable) with respect to the initial data and the source term data for gL1 and gL2 methods. Furthermore, if $\mathcal{Z}^{-1}(z)$ is a concave function, then the numerical scheme (21) is stable with the gL2-1 $_\sigma$ method.*

Theorem 4 (Convergence of FD-based scheme (21), see [81,86,87]). *Assume that P_z is a uniform z mesh and the solution $u(x, \mathcal{Z}^{-1}(z)) \in C^{4,r}([a, b] \times [z(0), z(T)])$, i.e., $\frac{d^4}{dx^4} u(x, \mathcal{Z}^{-1}(z))$ and $\frac{d^r}{dz^r} u(x, \mathcal{Z}^{-1}(z))$ is continuous. Let u_j^n and $u(x_j, t_n)$ denote the numerical solution obtained from (21) and the exact solution of (3), respectively. We have*

- for the gL1 method ($r = 2$)

$$\max_{1 \leq j \leq M-1} |u_j^n - u(x_j, t_n)| = O(\tau_z^{2-\alpha} + h^2), \quad 1 \leq n \leq N;$$

- for the gL2 method ($r = 3$)

$$\sqrt{\tau_z h \sum_{n=2}^N \sum_{j=1}^{M=1} |u_j^n - u(x_j, t_n)|^2} = O(\tau_z^{3-\alpha} + h^2), \quad 2 \leq n \leq N;$$

- for the gL2-1 $_{\sigma}$ method ($r = 3$)

$$\max_{1 \leq j \leq M-1} |u_j^n - u(x_j, t_n)| = O(\tau_z^2 + h^2), \quad 1 \leq n \leq N.$$

Remark 8. We note that the rigorous analysis of the stability and convergence of the fully discrete numerical scheme (21) relies on energy estimate and the monotonic property of the coefficients $\omega_{n,k}^*$. We can numerically observe high-order accuracy for the gL1-2 method. However, since the monotonicity of the coefficients does not hold for the gL1-2 method, it is challenging to establish the stability and convergence of this method under an energy estimate framework.

Remark 9. One can derive corresponding results for the generalized convolution quadrature method (18) using techniques from [83–85].

3.4.2. Compact Finite Difference (CFD) Method

Next, we present the fully discrete scheme based on the compact finite difference (CFD) method. Similarly to finite difference method, the discretization of (3) is considered at the point $(x_j, t_{n-1+\gamma})$, where $\gamma = 1$ or σ ($\sigma = 1 - \frac{\alpha}{2}$). Different from the finite difference method that applies approximations directly, the TDCFD operator H is applied first. From (3), this leads to

$$\begin{aligned} H {}^C D_{t;[z(t),1]}^{\alpha} u(x_j, t_{n-1+\gamma}) = & (1 - \gamma) H \mathcal{L} u(x_j, t_{n-1}) + \gamma H \mathcal{L} u(x_j, t_n) + \gamma(1 - \gamma) O(\tau_z^2) \\ & + H f_j^{n-1+\gamma}. \end{aligned}$$

Then, applying the compact finite difference approximation (20) of $\mathcal{L}$ and the generalized interpolation method (14) for ${}^C D_{t;[z(t),1]}^{\alpha} u(x_j, t_{n-1+\gamma})$ gives

$$\begin{aligned} & \frac{1}{\Gamma(2-\alpha)} \sum_{k=0}^{n-1} \omega_{n,k}^* \delta_z H u^{k+\frac{1}{2}}(x_j) + O(\tau_z^{\beta}) \\ = & (1 - \gamma) \left[\frac{1}{h} \left(\psi_{j+\frac{1}{2}}^{n-1} \delta_x u_{j+\frac{1}{2}}^{n-1} - \psi_{j-\frac{1}{2}}^{n-1} \delta_x u_{j-\frac{1}{2}}^{n-1} \right) - H q_j^{n-1} u_j^{n-1} \right] \\ & + \gamma \left[\frac{1}{h} \left(\psi_{j+\frac{1}{2}}^n \delta_x u_{j+\frac{1}{2}}^n - \psi_{j-\frac{1}{2}}^n \delta_x u_{j-\frac{1}{2}}^n \right) - H q_j^n u_j^n \right] + H f_j^{n-1+\gamma} + \gamma(1 - \gamma) O(\tau_z^2) + O(h^4). \end{aligned}$$

Once again, it is clear from the above formula that even if $\beta > 2$ (for example, when $\beta = 3 - \alpha$), the resulting method can only achieve $O(\tau_z^2)$ for $\gamma = \sigma$. After omitting small terms, we obtain the fully discrete scheme of (3) based on compact finite difference method, as follows

$$\begin{aligned} \frac{1}{\Gamma(2-\alpha)} \sum_{k=0}^{n-1} \omega_{n,k}^* \delta_z H u^{k+\frac{1}{2}}(x_j) = & (1 - \gamma) \left[\frac{1}{h} \left(\psi_{j+\frac{1}{2}}^{n-1} \delta_x u_{j+\frac{1}{2}}^{n-1} - \psi_{j-\frac{1}{2}}^{n-1} \delta_x u_{j-\frac{1}{2}}^{n-1} \right) - H q_j^{n-1} u_j^{n-1} \right] \\ & + \gamma \left[\frac{1}{h} \left(\psi_{j+\frac{1}{2}}^n \delta_x u_{j+\frac{1}{2}}^n - \psi_{j-\frac{1}{2}}^n \delta_x u_{j-\frac{1}{2}}^n \right) - H q_j^n u_j^n \right] + H f_j^{n-1+\gamma}. \quad (22) \end{aligned}$$

Similar to Theorems 3 and 4, we obtain the following stability and convergence results for the gL1, gL2 and gL2-1 $_{\sigma}$ methods.

Theorem 5 (Stability of CFD-based scheme (22); see [81,86,87]). *If P_z is uniformly distributed, then the numerical scheme (22) is robust (or stable) with respect to the initial data and the source term data for the gL1 and gL2 methods. Furthermore, if $\mathcal{Z}^{-1}(z)$ is a concave function, then the numerical scheme (22) is stable with the gL2-1 $_{\sigma}$ method.*

Theorem 6 (Convergence of CFD-based scheme (22); see [81,86,87]). *Assume that P_z is a uniform z mesh and the solution $u(x, \mathcal{Z}^{-1}(z)) \in C^{4,r}([a, b] \times [z(0), z(T)])$, i.e., $\frac{d^4}{dz^4} u(x, \mathcal{Z}^{-1}(z))$ and $\frac{d^r}{dz^r} u(x, \mathcal{Z}^{-1}(z))$, is continuous. Let u_j^n and $u(x_j, t_n)$ denote the numerical solution obtained from (22) and the exact solution of (3), respectively. We have*

- for the gL1 method ($r = 2$)

$$\max_{1 \leq j \leq M-1} |u_j^n - u(x_j, t_n)| = O(\tau_z^{2-\alpha} + h^4), \quad 1 \leq n \leq N;$$

- for the gL2 method ($r = 3$)

$$\sqrt{\tau_z h \sum_{n=2}^N \sum_{j=1}^{M-1} |u_j^n - u(x_j, t_n)|^2} = O(\tau_z^{3-\alpha} + h^4), \quad 2 \leq n \leq N;$$

- for the gL2-1 $_{\sigma}$ method ($r = 3$)

$$\max_{1 \leq j \leq M-1} |u_j^n - u(x_j, t_n)| = O(\tau_z^2 + h^4), \quad 1 \leq n \leq N.$$

Remark 10. Remarks 8 and 9 are still valid for the compact finite difference method, noting that in this case, fourth-order accuracy is obtained in the spatial dimension.

To summarize, in Section 3.4, we have shown how to derive the fully discrete schemes of (3) by employing the approximation of ${}_0^C D_{t;[z(t),1]}^{\alpha} u(x, t)$ based on the generalized interpolation method and the approximation of $\mathcal{L}$ discussed in Sections 3.1 and 3.3, respectively. This results in the fully discrete schemes (21) and (22). The fully discrete schemes utilizing the generalized convolution quadrature method (see Section 3.2) can be similarly derived.

Typically, the fully discrete scheme that is based on the finite difference method gives $O(h^2)$ in the spatial dimension, while employing the compact finite difference method may improve the spatial convergence to $O(h^4)$. This can be easily seen from the above derivation. We have presented the stability and convergence of the fully discrete schemes (21) and (22) in Theorems 3–6; more details can be found in [35,81,82,85–87,96–98]. Lastly, we note that the analysis of the fully discrete scheme based on the compact finite difference method is challenging for general $p(x, t)$; see the discussion in [81].

4. Numerical Experiment

In this section, we shall present some illustrative numerical results of the fully discrete schemes in Section 3.4. For this purpose, we shall demonstrate using the following example. Note that we only consider the compact finite difference method-based schemes here and leave the finite difference method-based schemes for interested readers.

Example 1 ([81]). *Examine the problem (3) with $a = 0$, $b = 1$, $T = 1$, $\psi(x) = 0$, $\phi_1(t) = t^{\gamma}$, $\phi_2(t) = et^{\gamma}$, $p(x, t) = 2 - \cos(xt)$, $q(x, t) = 1 - \sin(xt)$, and*

$$f(x, t) = e^x \left\{ \frac{\Gamma(\frac{\gamma}{\beta} + 1)}{\Gamma(\frac{\gamma}{\beta} + 1 - \alpha)} t^{\gamma - \beta\alpha} - t^{\gamma} [1 - \cos(xt) + (1 + t) \sin(xt)] \right\},$$

where $\gamma \geq \alpha\beta > 0$. We consider two cases:

Case A. Take the scale function $z(t) = t^\beta$ ($\beta \geq 1$), the exact solution is known to be $u(x, t) = t^\gamma e^x$.

Case B. Take the scale function $z(t) = \frac{1}{2}(t + t^2)$, $\beta = 1.5$, $\gamma = 5$, the exact solution is unknown.

In the experiment, we evaluate the *maximum absolute error* (MAE) when $t = t_N$, denoted by

$$e_{M,N} := \max_{1 \leq j \leq M-1} |u_j^N - U_j^N|,$$

where $\{U_j^n\}$ refers to the exact (or reference) solution and $\{u_j^n\}$ denotes the numerical solution, respectively. The corresponding temporal and spatial convergence orders are symbolized by

$$\mathcal{O}_t := \log_2 \frac{e_{M,N}}{e_{M,2N}} \quad \text{and} \quad \mathcal{O}_s := \log_2 \frac{e_{M,N}}{e_{2M,N}},$$

respectively.

Remark 11. Though some methods (e.g., gL1-2) do not have theoretical analysis and some theoretical results (e.g., gL2) are not in terms of maximum norm, we present only the results in terms of maximum absolute errors to show some insights. For other discrete norms, see [81] for the gL2 method and [83–85] for the gWSGL method.

Remark 12. We fix $\alpha = 0.2$ and vary β, γ for different purposes. The mesh $P_t = \{t_n\}$ is generated to ensure that $P_z = \{z_n\}$ conforms to either a uniform z mesh ($r = 1$) or a graded z mesh ($r > 1$):

$$z_n = z(0) + \left(\frac{n}{N}\right)^r z(T), \quad t_n = \mathcal{Z}^{-1}(z_n), \quad 0 \leq n \leq N.$$

4.1. Numerical Results Using Generalized Interpolation Method and CFD

In this section, we shall present numerical results for the fully discrete scheme (22), which is constructed by using the generalized interpolation type method (14) and compact finite difference method in the temporal and spatial dimensions, respectively. Note that for the gL2 method, we need to compute u_j^1 in advance. To do this, we shall apply gL1 approximation on graded z mesh [27] so that we can obtain an accurate result in the first step. Other than u_j^1 , the rest of u_j^n will be computed using uniform z mesh unless otherwise specified.

First, we fix $M = 400$ and vary N to compute maximum absolute errors and the corresponding temporal convergence order $\mathcal{O}_t$, using the gL1, gL1-2, gL2-1 $_\sigma$ and gL2 methods in (22) for Cases A and B. Since the convergence order varies significantly for different methods, we may need to deploy different N for different methods in order to observe the convergence order. Specifically,

- Case A: For the smooth case $\beta = 1.5$, $\gamma = 5$, we set $N = 1000, 2000, 4000$ for the gL1 method and $N = 200, 400, 800$ for the rest of the methods. For the non-smooth case $\beta = 1.5$, $\gamma = 0.3$, we set $N = 20, 40, 80$ for uniform z mesh and graded z mesh ($r = (2 - \alpha)/0.9$ for gL1 and $r = (3 - \alpha)/0.9$ for other methods).
- Case B: The exact solution is unknown in this case. We take $N = 10,000$, $M = 400$ to compute a reference solution, and deploy $N = 100, 200, 400$ for all methods.

The results are presented in Table 1. It is observed that if the solution is smooth, we obtain the expected temporal convergence orders (i.e., $2 - \alpha$ for gL1, $3 - \alpha$ for gL1-2, 2 for gL2-1 $_\sigma$ and $3 - \alpha$ for gL2) for both Cases A and B. If the solution is not smooth, then we observe the order reduction for uniform z mesh. As demonstrated in Remark 7, it can be tackled by graded z mesh that is also presented in Table 1.

Table 1. Errors and temporal convergence orders when $M = 400$.

Method	$\beta = 1.5, \gamma = 5$				Case A: $\beta = 1.5, \gamma = 0.3$			
	Case A		Case B		Uniform z Mesh		Graded z Mesh	
	$e_{M,N}$	$\mathcal{O}_t$	$e_{M,N}$	$\mathcal{O}_t$	$e_{M,N}$	$\mathcal{O}_t$	$e_{M,N}$	$\mathcal{O}_t$
gL1	5.193×10^{-7}	-	3.233×10^{-6}	-	3.206×10^{-4}	-	6.031×10^{-5}	-
	1.534×10^{-7}	1.76	9.766×10^{-7}	1.73	1.402×10^{-4}	1.19	1.722×10^{-5}	1.81
	4.510×10^{-8}	1.77	2.919×10^{-7}	1.74	6.204×10^{-5}	1.18	4.936×10^{-6}	1.80
gL1-2	3.320×10^{-8}	-	2.536×10^{-8}	-	2.286×10^{-4}	-	2.495×10^{-5}	-
	4.921×10^{-9}	2.75	3.775×10^{-9}	2.75	1.024×10^{-4}	1.16	3.265×10^{-6}	2.93
	7.224×10^{-10}	2.77	5.580×10^{-10}	2.76	4.593×10^{-5}	1.16	4.714×10^{-7}	2.79
gL2-1 $_{\sigma}$	1.608×10^{-6}	-	2.818×10^{-7}	-	2.327×10^{-4}	-	4.055×10^{-5}	-
	4.040×10^{-7}	1.99	7.169×10^{-8}	1.97	1.019×10^{-4}	1.19	9.487×10^{-6}	2.10
	1.013×10^{-7}	2.00	1.810×10^{-8}	1.99	4.513×10^{-5}	1.17	2.293×10^{-6}	2.05
gL2	3.320×10^{-8}	-	2.536×10^{-8}	-	1.480×10^{-4}	-	2.521×10^{-5}	-
	4.920×10^{-9}	2.75	3.775×10^{-9}	2.75	6.604×10^{-5}	1.16	3.297×10^{-6}	2.93
	7.224×10^{-10}	2.77	5.580×10^{-10}	2.76	2.934×10^{-5}	1.17	4.193×10^{-7}	2.98

Next, we turn to the spatial convergence order for both Cases A and B under smoothness assumption ($\gamma = 5, \beta = 1.5$). We consider uniform z mesh only and fix $N = 20,000$. To obtain a reference solution for Case B, we use $N = 20,000, M = 400$. For both cases, we set $M = 5, 10, 20$. Obviously, from Table 2, it is found that the expected fourth-order accuracy holds for all cases and all methods, which is consistent with the theoretical results in Theorem 6.

Table 2. Errors and spatial convergence orders when $N = 20,000$.

	gL1		gL1-2		gL2-1 $_{\sigma}$		gL2	
	$e_{M,N}$	$\mathcal{O}_s$	$e_{M,N}$	$\mathcal{O}_s$	$e_{M,N}$	$\mathcal{O}_s$	$e_{M,N}$	$\mathcal{O}_s$
Case A	6.633×10^{-6}	-	6.635×10^{-6}	-	6.635×10^{-6}	-	6.635×10^{-6}	-
	4.087×10^{-7}	4.02	4.113×10^{-7}	4.01	4.111×10^{-7}	4.01	4.113×10^{-7}	4.01
	2.324×10^{-8}	4.14	2.565×10^{-8}	4.00	2.549×10^{-8}	4.01	2.565×10^{-8}	4.00
Case B	1.424×10^{-7}	-	1.424×10^{-7}	-	1.424×10^{-7}	-	1.424×10^{-7}	-
	8.908×10^{-9}	4.00	8.909×10^{-9}	4.00	8.909×10^{-9}	4.00	8.909×10^{-9}	4.00
	5.567×10^{-10}	4.00	5.570×10^{-10}	4.00	5.570×10^{-10}	4.00	5.570×10^{-10}	4.00

4.2. Numerical Results Using Generalized Convolution Quadrature Method and CFD

In this section, we shall present numerical results for the fully discrete scheme constructed by using the generalized convolution quadrature type method (18) and compact finite difference method in the temporal and spatial dimensions, respectively. Let $\beta = 1.5, \gamma = 5$. Note that for $s = 3, 4$, we need to compute u_j^1 or u_j^2 in advance before starting the fully discrete scheme. We use the lower-order method to compute these values. To be specific, for $s = 3$ we compute u_j^1 using method $s = 2$, while for $s = 4$ we compute u_j^1 using method $s = 2$ and compute u_j^2 using method $s = 3$. As illustrated before, we may vary N, M differently for different s in order to obtain the desired convergence orders. Specifically,

- Case A: We set $M = 200$ and $N = 20, 40, 80$ to compute temporal convergence orders, and set $N = 10,000$ and $M = 5, 10, 20$ to compute spatial convergence orders.
- Case B: The reference solution is calculated using $N = 10,000, M = 400$. Subsequently, we set $M = 400$ and $N = 10, 20, 40$ to obtain the temporal convergence orders, and let $N = 10,000$ and $M = 5, 10, 20$ to compute the spatial convergence orders.

The results are presented in Table 3. Obviously, the convergence order is $O(\tau_z^s + h^4)$, which is consistent with the theoretical results.

Table 3. Errors , temporal and spatial convergence orders.

s	Case A		Case B		Case A		Case B	
	$e_{M,N}$	$\mathcal{O}_t$	$e_{M,N}$	$\mathcal{O}_t$	$e_{M,N}$	$\mathcal{O}_s$	$e_{M,N}$	$\mathcal{O}_s$
s = 2	1.545×10^{-4}	-	6.900×10^{-5}	-	6.635×10^{-6}	-	1.424×10^{-7}	-
	3.916×10^{-5}	1.98	1.772×10^{-5}	1.96	4.106×10^{-7}	4.01	8.909×10^{-9}	4.00
	9.857×10^{-6}	1.99	4.484×10^{-6}	1.98	2.505×10^{-8}	4.03	5.573×10^{-10}	4.00
s = 3	5.708×10^{-6}	-	5.132×10^{-6}	-	6.635×10^{-6}	-	1.424×10^{-7}	-
	7.159×10^{-7}	3.00	6.337×10^{-7}	3.02	4.113×10^{-7}	4.01	8.908×10^{-9}	4.00
	8.963×10^{-8}	3.00	7.871×10^{-8}	3.01	2.565×10^{-8}	4.00	5.566×10^{-10}	4.00
s = 4	3.623×10^{-8}	-	9.554×10^{-8}	-	6.635×10^{-6}	-	1.424×10^{-7}	-
	2.168×10^{-9}	4.06	6.362×10^{-9}	3.91	4.113×10^{-7}	4.01	8.908×10^{-9}	4.00
	1.303×10^{-10}	4.06	4.045×10^{-10}	3.98	2.565×10^{-8}	4.00	5.566×10^{-10}	4.00

5. Future Prospects

In this section, we shall propose some future investigations based on the above discussions and recent developments in models and numerical methods.

5.1. Generalized Time Fractional Models

So far, we have mainly summarized numerical methods for generalized time fractional models from the mathematical perspective. The best convergence order achieved is $O(\tau_z^4)$ for the smooth solution of the linear problem [84]. In applications, we may need to derive high order methods for linear and nonlinear problems with smooth as well as non-smooth solutions. It is known that these issues have been well addressed for $z(t) = t$ and $w(t) = 1$; see [22,24,25,37]. Using the aforementioned techniques, we may extend these methods to the generalized problems. On the other hand, generalized time fractional models from the application perspective [4] are very important in describing many phenomena in nature; however the existing methods are rather scarce. Therefore, it is both necessary and meaningful to propose high-order methods for this type of generalized fractional models.

5.2. Generalized Space Fractional Models

Time fractional models are typically related to the subdiffusion process, which is one of the anomalous diffusion processes. There is another anomalous diffusion process called super diffusion that typically results in space fractional models [3,4,7,16,17]. This type of fractional model has also been investigated extensively in the literature; see [102–105] for the finite element method, [106–109] for the finite difference method, [110] for the spectral collocation method, and the references therein. Amongst them, the fractional Laplacian and tempered fractional Laplacian [3,16,17] are two widely used operators in the models. Note that these two operators are actually the infinitesimal generator of the Lévy process and tempered Lévy process [3,17] that are widely applied to model phenomena at the microscopic level. One may expect a generalized space fractional model of which the generator is a more general stochastic process. Thus, such a model can be used to describe a variety of phenomena in a unified way. Also, efficient numerical methods are needed to simulate the trajectories of the particle and to observe its properties.

5.3. Deep Learning Based Method

Recently, a deep learning based-method has emerged to reduce the computation cost, especially for high-dimensional problems. The basic frameworks of deep learning-based methods are PINN [111], DRM [112], WAN [113], and BSDE [114]. Most other methods can be categorized into one of these frameworks. The generalized time fractional operator is a non-local operator and the computation of it is expensive. Therefore, it is necessary to reduce the computation cost. Hopefully, we may apply deep learning to achieve this

objective. There are some related pioneer works on classical fractional derivative [115,116]. One may apply these to tackle generalized time fractional derivatives and then solve the generalized time fractional models numerically. As for generalized space fractional models, they can be both high dimensional and non-local. Hence, deep learning methods become a natural and inevitable choice. There are some existing works [115,117–121] on this topic as well. It is also possible to extend to generalized space fractional operators.

6. Conclusions

In this paper, we first present the derivation of the generalized fractional models from two perspectives—mathematical and application. Next, to solve a class of generalized time fractional equations, some fully discrete numerical schemes are constructed based on the approximation of the generalized Caputo time fractional derivative, coupled with the approximation of the spatial derivative terms in the model. There are two methods for each type of approximation, namely, generalized interpolation method or generalized convolution quadrature method for the approximation of the generalized Caputo time fractional derivative; finite difference method or compact finite difference method for the approximation of the spatial derivative terms. Meanwhile, possible extensions are presented based on the current progress of classical fractional problems and its relation with generalized fractional models. Some experiments are also conducted to illustrate the numerical performance and convergence of the fully discrete schemes discussed. Finally, we propose some future research prospects of the generalized fractional models from the current framework and recent progress in scientific computing.

Author Contributions: Methodology, X.L. and P.J.Y.W.; validation, X.L. and P.J.Y.W., formal analysis, X.L. and P.J.Y.W.; investigation, X.L. and P.J.Y.W.; writing—original draft preparation, X.L.; writing—review and editing, P.J.Y.W. All authors have read and agreed to the published version of the manuscript.

Funding: This research receives no external funding.

Data Availability Statement: No new data were created or analyzed in this study.

Acknowledgments: The authors would like to thank the reviewers whose comments have helped to improve the paper.

Conflicts of Interest: The authors declare no conflicts of interest.

References

1. Diethelm, K. *The Analysis of Fractional Differential Equations*; Springer Science & Business Media: Berlin/Heidelberg, Germany, 2010.
2. Podlubny, I. *Fractional Differential Equations: An Introduction to Fractional Derivatives, Fractional Differential Equations, to Methods of Their Solution and Some of Their Applications*; Elsevier: Amsterdam, The Netherlands, 1998.
3. Deng, W. Anomalous and nonergodic multiscale modeling, analyses, and algorithms. *Sci. Sin. Math.* **2023**, *53*, 1–29. (In Chinese) [[CrossRef](#)]
4. Deng, W.; Hou, R.; Wang, W.; Xu, P. *Modeling Anomalous Diffusion: From Statistics to Mathematics*; World Scientific: Singapore, 2020.
5. Hilfer, R. *Applications of Fractional Calculus in Physics*; World Scientific: Singapore, 2000.
6. Uchaikin, V.; Sibatov, R. *Fractional Kinetics in Space: Anomalous Transport Models*; World Scientific: Singapore, 2017.
7. Metzler, R.; Klafter, J. The random walk's guide to anomalous diffusion: A fractional dynamics approach. *Phys. Rep.* **2000**, *339*, 1–77. [[CrossRef](#)]
8. Mainardi, F. *Fractional Calculus: Some Basic Problems in Continuum and Statistical Mechanics*; Springer: Berlin/Heidelberg, Germany, 1997.
9. Kilbas, A.A.; Srivastava, H.M.; Trujillo, J.J. *Theory and Applications of Fractional Differential Equations*; Elsevier: Berlin/Heidelberg, Germany, 2006.
10. Noeiaghdam, S.; Sidorov, D. Caputo-Fabrizio Fractional Derivative to Solve the Fractional Model of Energy Supply-Demand System. *Math. Model. Eng. Probl.* **2020**, *7*, 359–367. [[CrossRef](#)]

11. Loverro, A. Fractional Calculus: History, Definitions and Applications for the Engineer. In *Rapport Technique*; Univeristy of Notre Dame: Department of Aerospace and Mechanical Engineering; Notre Dame, IN, USA, 2004; pp. 1–28.
12. Kolwankar, K.; Gangal, A. Fractional differentiability of nowhere differentiable functions and dimensions. *Chaos Interdiscip. J. Nonlinear Sci.* **1996**, *6*, 505–513. [\[CrossRef\]](#)
13. Nishimoto, K. *An Essence of Nishimoto's Fractional Calculus (Calculus in the 21st Century): Integrations and Differentiations of Arbitrary Order*; Descartes Press Company: Waterloo, ON, USA, 1991.
14. Chen, M.; Deng, W. Fourth order accurate scheme for the space fractional diffusion equations. *SIAM J. Numer. Anal.* **2014**, *52*, 1418–1438. [\[CrossRef\]](#)
15. Zhang, Z.; Deng, W.; Karniadakis, G. A Riesz basis Galerkin method for the tempered fractional Laplacian. *SIAM J. Numer. Anal.* **2018**, *56*, 3010–3039. [\[CrossRef\]](#)
16. Lischke, A.; Pang, G.; Gulian, M.; Song, F.; Glusa, C.; Zheng, X.; Mao, Z.; Cai, W.; Meerschaert, M.M.; Ainsworth, M.; et al. What is the fractional Laplacian? A comparative review with new results. *J. Comput. Phys.* **2020**, *404*, 109009. [\[CrossRef\]](#)
17. Deng, W.; Li, B.; Tian, W.; Zhang, P. Boundary problems for the fractional and tempered fractional operators. *Multiscale Model. Simul.* **2018**, *16*, 125–149. [\[CrossRef\]](#)
18. Kubica, A.; Yamamoto, M. Initial-boundary value problems for fractional diffusion equations with time-dependent coefficients. *Fract. Calc. Appl. Anal.* **2018**, *21*, 276–311. [\[CrossRef\]](#)
19. Sakamoto, K.; Yamamoto, M. Initial value/boundary value problems for fractional diffusion-wave equations and applications to some inverse problems. *J. Math. Anal. Appl.* **2011**, *382*, 426–447. [\[CrossRef\]](#)
20. Deng, W.; Li, B.; Qian, Z.; Wang, H. Time discretization of a tempered fractional Feynman–Kac equation with measure data. *SIAM J. Numer. Anal.* **2018**, *56*, 3249–3275. [\[CrossRef\]](#)
21. Nie, D.; Deng, W. A Unified Convergence Analysis for the Fractional Diffusion Equation Driven by Fractional Gaussian Noise with Hurst Index $H \in (0, 1)$. *SIAM J. Numer. Anal.* **2022**, *60*, 1548–1573. [\[CrossRef\]](#)
22. Jin, B.; Lazarov, R.; Zhou, Z. Two fully discrete schemes for fractional diffusion and diffusion-wave equations with nonsmooth data. *SIAM J. Sci. Comput.* **2016**, *38*, A146–A170. [\[CrossRef\]](#)
23. Jin, B.; Lazarov, R.; Zhou, Z. Numerical methods for time-fractional evolution equations with nonsmooth data: A concise overview. *Comput. Methods Appl. Mech. Engrg.* **2019**, *346*, 332–358. [\[CrossRef\]](#)
24. Jin, B.; Li, B.; Zhou, Z. An analysis of the Crank–Nicolson method for subdiffusion. *IMA J. Numer. Anal.* **2018**, *38*, 518–541. [\[CrossRef\]](#)
25. Jin, B.; Li, B.; Zhou, Z. Numerical analysis of nonlinear subdiffusion equations. *SIAM J. Numer. Anal.* **2018**, *56*, 1–23. [\[CrossRef\]](#)
26. Stynes, M. Too much regularity may force too much uniqueness. *Fract. Calc. Appl. Anal.* **2016**, *19*, 1554–1562. [\[CrossRef\]](#)
27. Stynes, M.; O’Riordan, E.; Gracia, J. Error analysis of a finite difference method on graded meshes for a time-fractional diffusion equation. *SIAM J. Numer. Anal.* **2017**, *55*, 1057–1079. [\[CrossRef\]](#)
28. Cao, J.; Xu, W. Adaptive-coefficient finite difference frequency domain method for time fractional diffusive-viscous wave equation arising in geophysics. *Appl. Math. Lett.* **2025**, *160*, 109337. [\[CrossRef\]](#)
29. Jin, B.; Lazarov, R.; Zhou, Z. An analysis of the L1 scheme for the subdiffusion equation with nonsmooth data. *IMA J. Numer. Anal.* **2016**, *36*, 197–221. [\[CrossRef\]](#)
30. Kopteva, N.; Meng, X. Error analysis for a fractional-derivative parabolic problem on quasi-graded meshes using barrier functions. *SIAM J. Numer. Anal.* **2020**, *58*, 1217–1238. [\[CrossRef\]](#)
31. Liao, H.L.; Li, D.; Zhang, J. Sharp error estimate of the nonuniform L1 formula for linear reaction-subdiffusion equations. *SIAM J. Numer. Anal.* **2018**, *56*, 1112–1133. [\[CrossRef\]](#)
32. Sun, Z.Z.; Wu, X. A fully discrete difference scheme for a diffusion-wave system. *Appl. Numer. Math.* **2006**, *56*, 193–209. [\[CrossRef\]](#)
33. Alikhanov, A.A. A new difference scheme for the time fractional diffusion equation. *J. Comput. Phys.* **2015**, *280*, 424–438. [\[CrossRef\]](#)
34. Alikhanov, A.; Huang, C. A high-order L2 type difference scheme for the time-fractional diffusion equation. *Appl. Math. Comput.* **2021**, *411*, 126545. [\[CrossRef\]](#)
35. Alikhanov, A.; Huang, C. A class of time-fractional diffusion equations with generalized fractional derivatives. *J. Comput. Appl. Math.* **2022**, *414*, 114424. [\[CrossRef\]](#)
36. Chen, H.; Stynes, M. Error analysis of a second-order method on fitted meshes for a time-fractional diffusion problem. *J. Sci. Comput.* **2019**, *79*, 624–647. [\[CrossRef\]](#)
37. Kopteva, N. Error analysis of an L2-type method on graded meshes for a fractional-order parabolic problem. *Math. Comp.* **2021**, *90*, 19–40. [\[CrossRef\]](#)
38. Liao, H.L.; McLean, W.; Zhang, J. A second-order scheme with nonuniform time steps for a linear reaction-subdiffusion problem. *Commun. Comput. Phys.* **2021**, *30*, 567–601. [\[CrossRef\]](#)
39. Lv, C.; Xu, C. Error Analysis of A High Order Method for Time-Fractional Diffusion Equations. *SIAM J. Sci. Comput.* **2016**, *38*, A2699–A2724. [\[CrossRef\]](#)

40. Quan, C.; Wu, X. H1-norm stability and convergence of an L2-type method on nonuniform meshes for subdiffusion equation. *SIAM J. Numer. Anal.* **2023**, *61*, 2106–2132. [\[CrossRef\]](#)
41. Wang, Y.; Ren, L. A high-order L2-compact difference method for Caputo-type time-fractional sub-diffusion equations with variable coefficients. *Appl. Math. Comput.* **2019**, *342*, 71–93. [\[CrossRef\]](#)
42. Cao, J.X.; Li, C.P.; Chen, Y.Q. High-order approximation to Caputo derivatives and Caputo-type advection–diffusion equations (II). *Fract. Calc. Appl. Anal.* **2015**, *18*, 735–761. [\[CrossRef\]](#)
43. Li, H.; Cao, J.; Li, C. High-order approximation to Caputo derivatives and Caputo-type advection-diffusion equations (III). *J. Comput. Appl. Math.* **2016**, *299*, 159–175. [\[CrossRef\]](#)
44. Gao, G.; Sun, Z.; Zhang, H. A new fractional numerical differentiation formula to approximate the Caputo fractional derivative and its applications. *J. Comput. Phys.* **2014**, *259*, 33–50. [\[CrossRef\]](#)
45. Lubich, C. Discretized fractional calculus. *SIAM J. Math. Anal.* **1986**, *17*, 704–719. [\[CrossRef\]](#)
46. Lubich, C. Convolution quadrature and discretized operational calculus. I. *Numer. Math.* **1988**, *52*, 129–145. [\[CrossRef\]](#)
47. Lubich, C. Convolution quadrature and discretized operational calculus. II. *Numer. Math.* **1988**, *52*, 413–425. [\[CrossRef\]](#)
48. Lubich, C. Convolution quadrature revisited. *BIT Numer. Math.* **2004**, *44*, 503–514. [\[CrossRef\]](#)
49. Quarteroni, A.; Sacco, R.; Saleri, F. *Numerical Mathematics*; Springer Science & Business Media: Berlin/Heidelberg, Germany, 2010; Volume 37.
50. Cuesta, E.; Lubich, C.; Palencia, C. Convolution quadrature time discretization of fractional diffusion-wave equations. *Math. Comp.* **2006**, *75*, 673–696. [\[CrossRef\]](#)
51. Akrivis, G.; Chen, M.; Han, J.; Yu, F.; Zhang, Z. The variable two-step BDF method for parabolic equations. *BIT Numer. Math.* **2024**, *64*, 14. [\[CrossRef\]](#)
52. Li, Z.; Liao, H.L. Stability of variable-step BDF2 and BDF3 methods. *SIAM J. Numer. Anal.* **2022**, *60*, 2253–2272. [\[CrossRef\]](#)
53. Liao, H.L.; Tang, T.; Zhou, T. Discrete energy analysis of the third-order variable-step BDF time-stepping for diffusion equations. *J. Comput. Math.* **2023**, *41*, 325–344. [\[CrossRef\]](#)
54. Liao, H.L.; Zhang, Z. Analysis of adaptive BDF2 scheme for diffusion equations. *Math. Comp.* **2021**, *90*, 1207–1226. [\[CrossRef\]](#)
55. Pei, L.; Wei, Y.; Zhang, J. Unconditional optimal H1-norm error estimate and superconvergence analysis of a linearized nonconforming finite element variable-time-step BDF2 method for the nonlinear complex Ginzburg–Landau equation. *Commun. Nonlinear Sci. Numer. Simul.* **2024**, *138*, 108193. [\[CrossRef\]](#)
56. Tian, W.; Zhou, H.; Deng, W. A class of second order difference approximations for solving space fractional diffusion equations. *Math. Comp.* **2015**, *84*, 1703–1727. [\[CrossRef\]](#)
57. Akrivis, G.; Chen, M.; Yu, F. The weighted and shifted seven-step BDF method for parabolic equations. *IMA J. Numer. Anal.* **2024**, drae089. [\[CrossRef\]](#)
58. Agrawal, O.P. Some generalized fractional calculus operators and their applications in integral equations. *Fract. Calc. Appl. Anal.* **2012**, *15*, 700–711. [\[CrossRef\]](#)
59. Almeida, R. A Caputo fractional derivative of a function with respect to another function. *Commun. Nonlinear Sci. Numer. Simul.* **2017**, *44*, 460–481. [\[CrossRef\]](#)
60. Chen, Z.Q.; Deng, W.; Xu, P. Feynman–Kac Transform for Anomalous Processes. *SIAM J. Math. Anal.* **2021**, *53*, 6017–6047. [\[CrossRef\]](#)
61. Kilbas, A.; Marichev, O.; Samko, S. *Fractional Integrals and Derivatives (Theory and Applications)*; Gordon and Breach: Montreux, Switzerland, 1993.
62. De Oliveira, E.; Machado, J. A review of definitions for fractional derivatives and integral. *Math. Probl. Eng.* **2014**, *2014*, 238459. [\[CrossRef\]](#)
63. Abdeljawad, T. On conformable fractional calculus. *J. Comput. Appl. Math.* **2015**, *279*, 57–66. [\[CrossRef\]](#)
64. Khalil, R.; Al Horani, M.; Yousef, A.; Sababheh, M. A new definition of fractional derivative. *J. Comput. Appl. Math.* **2014**, *264*, 65–70. [\[CrossRef\]](#)
65. Atangana, A.; Doungmo Goufo, E. Extension of matched asymptotic method to fractional boundary layers problems. *Math. Probl. Eng.* **2014**, *2014*, 107535. [\[CrossRef\]](#)
66. Kiryakova, V. *Generalized Fractional Calculus and Applications*; CRC Press: Boca Raton, FL, USA, 1993.
67. Mathai, A.; Haubold, H. *Erdélyi-Kober Fractional Calculus: From a Statistical Perspective, Inspired by Solar Neutrino Physics*; Springer: Berlin/Heidelberg, Germany, 2018; Volume 31.
68. Pagnini, G. Erdélyi-Kober fractional diffusion. *Fract. Calc. Appl. Anal.* **2012**, *15*, 117–127. [\[CrossRef\]](#)
69. Plociniczak, L. Approximation of the Erdélyi-Kober operator with application to the time-fractional Porous medium equation. *SIAM J. Appl. Math.* **2014**, *74*, 1219–1237. [\[CrossRef\]](#)
70. Plociniczak, L.; Świtla, M. Numerical scheme for Erdélyi-Kober fractional diffusion equation using Galerkin–Hermite method. *Fract. Calc. Appl. Anal.* **2022**, *25*, 1651–1687. [\[CrossRef\]](#)

71. Luchko, Y.; Trujillo, J. Caputo-type modification of the Erdélyi-Kober fractional derivative. *Fract. Calc. Appl. Anal.* **2007**, *10*, 249–267.
72. Tawfik, A.M.; Abdelhamid, H.M. Generalized fractional diffusion equation with arbitrary time varying diffusivity. *Appl. Math. Comput.* **2021**, *410*, 126449. [[CrossRef](#)]
73. Agrawal, O. Generalized variational problems and Euler–Lagrange equations. *Comput. Math. Appl.* **2010**, *59*, 1852–1864. [[CrossRef](#)]
74. Xu, Y.; Agrawal, O. Models and numerical schemes for generalized van der Pol equations. *Commun. Nonlinear Sci. Numer. Simul.* **2013**, *18*, 3575–3589. [[CrossRef](#)]
75. Xu, Y.; Agrawal, O. Models and numerical solutions of generalized oscillator equations. *J. Vib. Acoust.* **2014**, *136*, 050903. [[CrossRef](#)]
76. Meerschaert, M.; Scheffler, H.P. Limit theorems for continuous-time random walks with infinite mean waiting times. *J. Appl. Probability* **2004**, *41*, 623–638. [[CrossRef](#)]
77. Chen, Z.Q. Time fractional equations and probabilistic representation. *Chaos Solitons Fractals* **2017**, *102*, 168–174. [[CrossRef](#)]
78. Gu, X.M.; Huang, T.Z.; Zhao, Y.L.; Lyu, P.; Carpentieri, B. A fast implicit difference scheme for solving the generalized time–space fractional diffusion equations with variable coefficients. *Numer. Methods Partial. Differ. Equ.* **2021**, *37*, 1136–1162. [[CrossRef](#)]
79. Khibiev, A.; Alikhanov, A.; Huang, C. A second-order difference scheme for generalized time-fractional diffusion equation with smooth solutions. *Comput. Methods Appl. Math.* **2024**, *24*, 101–117. [[CrossRef](#)]
80. Li, X.; Wong, P. Two new approximations for generalized Caputo fractional derivative and their application in solving generalized fractional sub-diffusion equations. *J. Appl. Math. Comput.* **2023**, *69*, 4689–4716. [[CrossRef](#)]
81. Li, X.; Wong, P.; Alikhanov, A. Numerical method for fractional sub-diffusion equation with space–time varying diffusivity and smooth solution. *J. Comput. Appl. Math.* **2025**, *464*, 116473. [[CrossRef](#)]
82. Xu, Y.; He, Z.; Agrawal, O.P. Numerical and analytical solutions of new generalized fractional diffusion equation. *Comput. Math. Appl.* **2013**, *66*, 2019–2029. [[CrossRef](#)]
83. Ding, Q.; Wong, P. A higher order numerical scheme for generalized fractional diffusion equations. *Internat. J. Numer. Methods Fluids* **2020**, *92*, 1866–1889. [[CrossRef](#)]
84. Ding, Q.; Wong, P. A new approximation for the generalized fractional derivative and its application to generalized fractional diffusion equation. *Numer. Methods Partial. Differ. Equ.* **2021**, *37*, 643–673. [[CrossRef](#)]
85. Li, X.; Wong, P. A gWSGL numerical scheme for generalized fractional sub-diffusion problems. *Commun. Nonlinear Sci. Numer. Simul.* **2020**, *82*, 104991. [[CrossRef](#)]
86. Li, X.; Wong, P. Generalized Alikhanov’s approximation and numerical treatment of generalized fractional sub-diffusion equations. *Commun. Nonlinear Sci. Numer. Simul.* **2021**, *97*, 105719. [[CrossRef](#)]
87. Li, X.; Wong, P. gL1 scheme for solving a class of generalized time-fractional diffusion equations. *Mathematics* **2022**, *10*, 1219. [[CrossRef](#)]
88. Cockburn, B.; Mustapha, K. A hybridizable discontinuous Galerkin method for fractional diffusion problems. *Numer. Math.* **2015**, *130*, 293–314. [[CrossRef](#)]
89. Mustapha, K.; McLean, W. Piecewise-linear, discontinuous Galerkin method for a fractional diffusion equation. *Numer. Algorithms* **2011**, *56*, 159–184. [[CrossRef](#)]
90. Mustapha, K.; McLean, W. Superconvergence of a discontinuous Galerkin method for fractional diffusion and wave equations. *SIAM J. Numer. Anal.* **2013**, *51*, 491–515. [[CrossRef](#)]
91. Xu, Q.; Hesthaven, J. Discontinuous Galerkin method for fractional convection-diffusion equations. *SIAM J. Numer. Anal.* **2014**, *52*, 405–423. [[CrossRef](#)]
92. Deng, W.; Hesthaven, J. Local Discontinuous Galerkin methods for fractional diffusion equations. *ESAIM Math. Model. Numer. Anal.* **2013**, *47*, 1845–1864. [[CrossRef](#)]
93. Harizanov, S.; Lazarov, R.; Margenov, S. A survey on numerical methods for spectral space-fractional diffusion problems. *Fract. Calc. Appl. Anal.* **2020**, *23*, 1605–1646. [[CrossRef](#)]
94. Hou, D.; Xu, C. A fractional spectral method with applications to some singular problems. *Adv. Comput. Math.* **2017**, *43*, 911–944. [[CrossRef](#)]
95. Zayernouri, M.; Karniadakis, G. Fractional spectral collocation method. *SIAM J. Sci. Comput.* **2014**, *36*, A40–A62. [[CrossRef](#)]
96. Kumar, K.; Pandey, R.; Sultana, F. Numerical schemes with convergence for generalized fractional integro-differential equations. *J. Comput. Appl. Math.* **2021**, *388*, 113318. [[CrossRef](#)]
97. Xu, Y.; He, Z.; Xu, Q. Numerical solutions of fractional advection-diffusion equations with a kind of new generalized fractional derivative. *Int. J. Comput. Math.* **2014**, *91*, 588–600. [[CrossRef](#)]
98. Kumar, K.; Pandey, A.; Pandey, R. High Order Numerical Scheme for Generalized Fractional Diffusion Equations. *Int. J. Appl. Comput. Math.* **2024**, *10*, 105. [[CrossRef](#)]

99. Kumari, S.; Pandey, R.; Agarwal, R. High-Order Approximation to Generalized Caputo Derivatives and Generalized Fractional Advection–Diffusion Equations. *Mathematics* **2023**, *11*, 1200. [\[CrossRef\]](#)
100. Shi, J.; Chen, M.; Yan, Y.; Cao, J. Correction of High-Order L_k Approximation for Subdiffusion. *J. Sci. Comput.* **2022**, *93*, 31. [\[CrossRef\]](#)
101. Sun, Z.Z. An unconditionally stable and $O(\tau^2 + h^4)$ order L_∞ convergent difference scheme for linear parabolic equations with variable coefficients. *Numer. Methods Partial. Differ. Equ.* **2001**, *17*, 619–631. [\[CrossRef\]](#)
102. Acosta, G.; Borthagaray, J. A fractional Laplace equation: Regularity of solutions and finite element approximations. *SIAM J. Numer. Anal.* **2017**, *55*, 472–495. [\[CrossRef\]](#)
103. Bonito, A.; Borthagaray, J.; Nocketto, R.; Otárola, E.; Salgado, A. Numerical methods for fractional diffusion. *Comput. Vis. Sci.* **2018**, *19*, 19–46. [\[CrossRef\]](#)
104. Borthagaray, J.; Nocketto, R. Constructive approximation on graded meshes for the integral fractional Laplacian. *Constr. Approx.* **2023**, *57*, 463–487. [\[CrossRef\]](#)
105. Faustmann, M.; Marcati, C.; Melenk, J.; Schwab, C. Exponential Convergence of FEM for the Integral Fractional Laplacian in Polygons. *SIAM J. Numer. Anal.* **2023**, *61*, 2601–2622. [\[CrossRef\]](#)
106. Han, R.; Wu, S. A monotone discretization for integral fractional Laplacian on bounded Lipschitz domains: Pointwise error estimates under Hölder regularity. *SIAM J. Numer. Anal.* **2022**, *60*, 3052–3077. [\[CrossRef\]](#)
107. Hao, Z.; Zhang, Z.; Du, R. Fractional Centered Difference Scheme for High-Dimensional Integral Fractional Laplacian. *J. Comput. Phys.* **2021**, *424*, 109851. [\[CrossRef\]](#)
108. Huang, Y.; Oberman, A. Numerical methods for the fractional Laplacian: A finite difference-quadrature approach. *SIAM J. Numer. Anal.* **2014**, *52*, 3056–3084. [\[CrossRef\]](#)
109. Huang, Y.; Oberman, A. Finite difference methods for fractional Laplacians. *arXiv* **2016**, arXiv:1611.00164. [\[CrossRef\]](#)
110. Antil, H.; Dondl, P.; Striet, L. Analysis of a Sinc-Galerkin method for the fractional Laplacian. *SIAM J. Numer. Anal.* **2023**, *61*, 2967–2993. [\[CrossRef\]](#)
111. Raissi, M.; Perdikaris, P.; Karniadakis, G. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *J. Comput. Phys.* **2019**, *378*, 686–707. [\[CrossRef\]](#)
112. E, W.; Yu, B. The deep Ritz method: A deep learning-based numerical algorithm for solving variational problems. *Commun. Math. Stat.* **2018**, *6*, 1–12. [\[CrossRef\]](#)
113. Zang, Y.; Bao, G.; Ye, X.; Zhou, H. Weak adversarial networks for high-dimensional partial differential equations. *J. Comput. Phys.* **2020**, *411*, 109409. [\[CrossRef\]](#)
114. Han, J.; Jentzen, A.; E, W. Solving high-dimensional partial differential equations using deep learning. *Proc. Nat. Acad. Sci. USA* **2018**, *115*, 8505–8510. [\[CrossRef\]](#)
115. Guo, L.; Wu, H.; Yu, X.; Zhou, T. Monte Carlo fPINNs: Deep learning method for forward and inverse problems involving high dimensional fractional partial differential equations. *Comput. Methods Appl. Mech. Engrg.* **2022**, *400*, 115523. [\[CrossRef\]](#)
116. Pang, G.; Lu, L.; Karniadakis, G. fPINNs: Fractional physics-informed neural networks. *SIAM J. Sci. Comput.* **2019**, *41*, A2603–A2626. [\[CrossRef\]](#)
117. Gu, Y.; Ng, M. Deep Ritz Method for the Spectral Fractional Laplacian Equation Using the Caffarelli–Silvestre Extension. *SIAM J. Sci. Comput.* **2022**, *44*, A2018–A2036. [\[CrossRef\]](#)
118. Gulian, M.; Raissi, M.; Perdikaris, P.; Karniadakis, G. Machine learning of space-fractional differential equations. *SIAM J. Sci. Comput.* **2019**, *41*, A2485–A2509. [\[CrossRef\]](#)
119. Hao, Z.; Park, M.; Cai, Z. Neural Network Method for Integral Fractional Laplace Equations. *East Asian J. Appl. Math.* **2022**, *13*, 95–118. [\[CrossRef\]](#)
120. Hu, Z.; Kawaguchi, K.; Zhang, Z.; Karniadakis, G. Tackling the Curse of Dimensionality in Fractional and Tempered Fractional PDEs with Physics-Informed Neural Networks. *arXiv* **2024**, arXiv:2406.11708. [\[CrossRef\]](#)
121. Zeng, L.; Wan, X.; Zhou, T. Adaptive Deep Density Approximation for Fractional Fokker–Planck Equations. *J. Sci. Comput.* **2023**, *97*, 68. [\[CrossRef\]](#)

Disclaimer/Publisher’s Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.