Generalized convolution quadrature for the fractional integral and fractional diffusion equations

J. Guo * M. Lopez-Fernandez†
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Abstract

We consider the application of the generalized Convolution Quadrature (gCQ) of the first order to approximate fractional integrals and associated fractional diffusion equations. The gCQ is a generalization of Lubich’s Convolution Quadrature (CQ) which allows for variable steps. In this paper we analyze the application of the gCQ to fractional integrals, with a focus on the low regularity case. It is well known that in this situation the original CQ presents an order reduction close to the singularity. The available theory for the gCQ does not cover this situation. Here we use a different expression for the numerical approximation and the associated error, which allows us to significantly relax the regularity requirements for the application of the gCQ method. In particular we are able to eliminate the a priori regularization step required in the original derivation of the gCQ. We show first order of convergence for a general time mesh under much weaker regularity requirements than previous results in the literature. We also prove that uniform first order convergence is achievable for a graded time mesh, which is appropriately refined close to the singularity, according to the order of the fractional integral and the regularity of the data. Then we study how to obtain full order of convergence for the application to linear fractional diffusion equations. An important advantage of the gCQ method is that it allows for a fast and memory reduced implementation. We outline how this algorithm can be implemented and illustrate our theoretical results with several numerical experiments.

Keywords: fractional integral, fractional differential equations, generalized convolution quadrature, variable steps, graded meshes.

AMS subject classifications: 65R20, 65L06, 65M15, 26A33, 35R11.

1 Introduction

We consider the evaluation of the fractional integral

$$\mathcal{I}^\alpha[f](t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t-s)^{\alpha-1} f(s) \, ds,$$

for a given function $f$, which can be vector-valued, and $\alpha \in (0,1)$. We will focus on the low regularity setting of $f(t) = O(t^\beta)$, as $t \to 0$, with

$$\beta > -1.$$
A standard discretization of (1) is obtained by Lubich’s Convolution Quadrature (CQ), either based on a linear multistep method, as originally proposed in [15], or based on a Runge-Kutta scheme [17, 2]. The original CQ method relies on the choice of a uniform time mesh \( t_n = nh \), for some fixed \( h > 0 \) and \( n = 0, \ldots, N \), with \( T = Nh \), and it is well known to suffer an order reduction if the zero-extension of the data \( f \) to \( t < 0 \) is non smooth enough, depending on \( \alpha, \beta \) and the order \( p \) of the chosen formula. This question has been thoroughly analyzed in the literature, starting from the introduction of the CQ itself in [15]. Specifically for the approximation of order \( p = 1 \), the theory in [15, Theorem 5.2, Corollary 3.2], guarantees order one only at a given time point and shows that the error deteriorates as \( t \to 0 \). For approximations of order higher than one, correction terms are needed in order to achieve the full maximal order at a given time point.

In this paper, we deduce \textit{a priori} error bounds for the application of the generalized Convolution Quadrature (gCQ) of the first order to (1) on an arbitrary time grid \( \Delta := 0 < t_1 < \cdots < t_N = T \), for \( N \geq 1 \). The gCQ method was first presented and analyzed in [11], where first order convergence is proven under strong regularity requirements on the extension of \( f \) to \( t < 0 \). The analysis in [11] is mostly oriented to the numerical approximation of hyperbolic retarded potentials and, thus, no regularity of the convolution kernel is assumed. CQ methods and also its generalization to variable steps, what we call gCQ, are based on a proper contour integral representation of the convolution and its numerical approximation. For convolution kernels which are not regular enough, such as those associated to the boundary integral formulation of many hyperbolic problems, this contour must be taken parallel to the imaginary axis [2, 11]. However, the kernel in (1) is sectorial, like those studied in [17]. Moreover, since the Laplace transform of the kernel \( t^{\alpha-1}/\Gamma(\alpha) \) is \( z^{-\alpha} \), which is analytic in the whole complex plane but the branch cut along the negative real axis, a specially convenient contour integral representation is possible in this case. In fact, in this case, the complex contour can be degenerated into the cut along the negative real axis and the integral representation ends up to be real [1]. This representation of both (1) and its numerical discretization by the gCQ method, allow us to show that the regularity hypotheses in [11] for the gCQ of the first order can be significantly relaxed. In particular, we are able to eliminate the a priori regularization step required by the original theory in [11]. To do this, we use special analytic representations of the Euler remainder (see Section 3) and perform a careful analysis of the integrated error. To be more precise, we notice that the original gCQ scheme, as presented in [11], for (1) must actually be applied to the regularized convolution

\[
\frac{1}{\Gamma(\alpha + 1)} \int_0^t (t - s)^\alpha f'(s) \, ds,
\]

which is equivalent to (1) only if \( f' \) is integrable and \( f(0) = 0 \). Moreover, the convergence proof in [11] requires essentially the extension to \( t < 0 \) of \( f \) to be of class \( C^3 \). In this paper we allow \( f \) to be an \( O(t^\beta) \), with \( \beta > -1 \), as \( t \to 0^+ \), and do not require any a priori regularization of (1) to apply the scheme, working directly with (1). This is a significant improvement of the existing theory and might open the way to further theoretical developments, both for higher order versions of the gCQ method, which allow for an analogous representation of the gCQ, see [1], and also for convolutions with more general sectorial kernels. Still, we consider the first order method to be relevant enough to be studied on its own in a low regularity setting like this.

The special representation of (1) has been recently used in [3] for a posteriori error analysis of both the L1 scheme and the gCQ of the first order. For the L1 method the maximal order of convergence is known to be \( 2 - \alpha \), higher than for the gCQ of the first order. In [3], the maximal order is shown to be achievable in the \( L^2 \) norm by using appropriate graded meshes based on the a posteriori error analysis. A posteriori
error formulas are derived also for the gCQ method of the first order, but the asymptotic analysis of them is not performed. The authors point indeed to the complicated a priori error analysis required for this. In this paper we address precisely this a priori error analysis and derive error bounds in the $L^\infty$ norm for the gCQ method of the first order. We obtain optimal error estimates of full first order for general meshes and, as a particular case, for appropriate graded meshes. By doing this, we fill an important gap in the theory of [11], for this application.

Efficient algorithms for both the L1 method and the CQ method with uniform time step are nowadays available for (1), see [7] and [1], respectively. For $N$ the total number of time steps, these algorithms are able to reduce the complexity from $O(N^2)$ to $O(N \log(N))$, and the memory requirements from $O(N)$ to $O(\log(N))$. For the implementation of the CQ this is known as fast and oblivious CQ [21]. For the gCQ, with variable time steps, similar gains are possible. In the present paper we focus mostly on the theoretical a priori analysis of the gCQ and only outline the corresponding algorithm, which combines the special quadratures developed in [12] for the gCQ with a generalization of the quadrature in [1] for the CQ. A careful theoretical analysis of the final complexity and memory requirements of the fast and oblivious gCQ algorithm for (1), is beyond the scope of this work, but several numerical results are displayed here in Section 6.

As we have already mentioned above, our analysis is performed on an arbitrary time grid but we consider with detail the particular choice of graded meshes, defined by

$$t_n = (n\tau)^\gamma, \quad \tau = \frac{T^{1/\gamma}}{N}, \quad n = 1, \ldots, N. \quad (4)$$

For (4) we derive the optimal value of the grading parameter $\gamma$ as a function of $\alpha$ and $\beta$ in order to achieve full order of convergence. Quite recently, other variable step schemes specific for subdiffusion equations have been proposed in the literature, based on the choice of graded meshes to deal with the singularity at the origin of the solution. On the one hand there are variable step versions of the L1 scheme on graded meshes [19, 22] and the more general analysis in [9]. We mention also a novel exponential convolution quadrature method in [8], designed for nonlinear subdiffusion problems which achieves optimal order of convergence on special graded time meshes. In the present paper we focus on the discretization of the fractional integral (1) on arbitrary time meshes, not necessarily graded ones, and the application to associated linear subdiffusion problems is derived from this. We can proceed this way thanks to the preservation of the composition rule of convolutions by the gCQ scheme, see Remark 2 and Section 4. Notice that other interesting applications involve memory terms of the type (1), such problems with transparent boundary conditions [18] or impedance boundary conditions [6], and for them the present analysis is also relevant.

The paper is organized as follows. In Section 2 we recall the definition of the generalized Convolution Quadrature method of the first order and the convergence result proven in [11] for its application to (1), which requires $f \in C^4(0, T)$ and the extension of $f$ to $t < 0$ to be of class $C^3$. In Section 3 we analyze the non smooth case $f = O(t^\beta)$, with $\beta > -1$. In Section 4 we address the application to fractional diffusion equations. Section 5 is devoted to implementation issues and numerical results are shown in Section 6.

2 Generalized Convolution Quadrature of the first order

We present the gCQ method for (1) in a different way to the derivation in [11], taking into account the specific properties of the convolution kernel $t^{\alpha-1}/\Gamma(\alpha)$. For this, we recall
the real integral representation formula of the convolution kernel

$$\frac{\Gamma(\alpha - 1)}{\Gamma(\alpha)} = \frac{\sin(\pi \alpha)}{\pi} \int_0^\infty x^{-\alpha} e^{-xt} dx,$$  \hspace{1cm} (5)

which has already been successfully used in [1] for the implementation of the original CQ. We then can write

$$I_\alpha[f](t) = \frac{\sin(\pi \alpha)}{\pi} \int_0^\infty x^{-\alpha} \int_0^t e^{-x(t-s)} f(s) ds \, dx$$

$$= \frac{\sin(\pi \alpha)}{\pi} \int_0^\infty x^{-\alpha} y(x, t) \, dx,$$  \hspace{1cm} (6)

with $y(x, t)$ the solution to the scalar ODE problem

$$\partial_t y(x, t) = -xy(x, t) + f(t), \quad \text{with} \quad y(x, 0) = 0, \quad x \in (0, \infty), \quad t \in (0, T].$$  \hspace{1cm} (7)

With this representation of the convolution kernel, the gCQ approximation of (1) is defined below.

**Definition 1.** For a given $N \geq 0$ and a sequence of time points

$$\Delta := 0 < t_1 < \cdots < t_N = T, \quad \text{with} \quad \tau_k := t_k - t_{k-1}, \quad k \geq 1,$$  \hspace{1cm} (8)

the generalized Convolution Quadrature approximation to (1) based on the implicit Euler method is given by

$$I_\alpha^n[f] = \frac{\sin(\pi \alpha)}{\pi} \int_0^\infty x^{-\alpha} y_n(x) \, dx,$$  \hspace{1cm} (9)

where $y_n(x)$ is the approximation of $y(x, t_n)$ in (7) given by the implicit Euler method, this is,

$$y_n(x) = \sum_{k=1}^n \tau_k \left( \prod_{j=k}^n \frac{1}{1 + \tau_j x} \right) f(t_k).$$  \hspace{1cm} (10)

We will write for short

$$I_\alpha^n[f] = \sum_{k=1}^n \omega_{n,k} f_k,$$  \hspace{1cm} (11)

with $f_k = f(t_k)$ and

$$\omega_{n,k} := \tau_k \frac{\sin(\pi \alpha)}{\pi} \int_0^\infty x^{-\alpha} \prod_{j=k}^n r(\tau_j x) \, dx, \quad r(x) := \frac{1}{1 + x},$$  \hspace{1cm} (12)

the gCQ weights. Notice that $r(x) = R(-x)$, with $R(z) = \frac{1}{1+z}$ the stability function of the implicit Euler method.

**Remark 2.** Our definition of the gCQ approximation (9) to (1) is equivalent to the one in [11], and thus inherits its properties, such as the preservation of the composition rule. More precisely, by using Lubich’s operational notation for one-sided convolutions [16]

$$(K(\partial_t)f)(t) := \int_0^t k(t-s)f(s) \, ds, \quad \text{with} \quad K = \mathcal{L}[k],$$  \hspace{1cm} (13)

it holds

$$K_2(\partial_t)K_1(\partial_t)f = (K_2 \cdot K_1)(\partial_t)f.$$  \hspace{1cm} (14)
Following the notation in [13], if we denote by $K(\partial^\Delta t)f$ the vector of approximations to $(K(\partial t)f)(t_j)$ on a general time grid

$$\Delta := 0 < t_1 < \cdots < t_N = T,$$

by the gCQ method, it is proven in [13, Section 5.2] that

$$K_2(\partial^\Delta t)K_1(\partial^\Delta t)f = (K_2 \cdot K_1)(\partial^\Delta t)f.$$  

(16)

This property is essential in many error proofs of CQ based schemes and will be used in Section 4 when discussing the application to subdiffusion equations.

In [11] a complex contour integral representation of the convolution kernel is used, which is derived from Bromwich inversion formula of the Laplace transform. Here we use the real integral representation of the kernel (5), which can actually be derived from deformation of the Bromwich contour, too, as explained in [1]. Our representation of the gCQ discretization for the fractional integral is both useful for the implementation of the method, see [1], and also for the error analysis in the low regularity setting, as we show in Section 3.

We recall here the convergence result proven in [11]. The gCQ method is originally defined for more general convolution problems

$$c(t) = \int_0^t k(t-s)f(s) \, ds.$$  

(17)

The kernel $k$ is assumed to be the inverse Laplace transform of a mapping $K(z)$, which is defined in a half plane $\text{Re } z \geq \sigma_0$ and grows algebraically as

$$|K(z)| \leq C|z|^\mu, \quad \text{Re } z \geq \sigma_0,$$

(18)

for some $C > 0$, $\mu \in \mathbb{R}$. The numerical approximation (9) is not valid in this more general case. Both regularization of the problem by differentiation of $f$, according to the value of $\mu$, and integration along a contour laying in the right half of the complex plane are in general required. For the case of (1), the following result follows from the theory in [11].

**Theorem 3** (Theorem 4.5 in [11]). Let $0 < \sigma_0 < \tau_{\text{max}}^{-1}$ with

$$\tau_{\text{max}} := \max_{1 \leq k \leq N} \{\tau_k\}.$$  

(19)

We assume that $f \in C^4([0,T])$ and $f^{(\ell)}(0) = 0$ for all $0 \leq \ell \leq 3$. We denote by $c_n$, for $1 \leq n \leq N$, the approximation of (17) by the gCQ method of the first order. Then, the error estimate holds

$$|c(t_n) - c_n| \leq C p_{\nu + \alpha}(\tau_{\text{max}}) \tau_{\text{max}} \left( \sum_{j=1}^n \frac{\tau_j + \tau_{j-1}}{2} e^{-\delta_0 t_{j-1}} \max_{\tau \in [t_{j-2}, t_j]} \left\| f^{(\ell)}(\tau) \right\|_D \right),$$

with

$$p_\nu (\tau_{\text{max}}) = \begin{cases} 
1 + \log \frac{1}{\tau_{\text{max}}}, & \text{if } \nu = 1, \\
1, & \text{if } \nu > 1.
\end{cases}$$

(20)

We are now able to relax these strong regularity requirements for the case of (1) by using the sectoriality of the Laplace transform $K(z) = z^{-\alpha}$, which is analytic in the whole complex plane cut by the negative real line.

Higher order versions of the gCQ based on Runge–Kutta methods have been proposed and analyzed in [13] for convolution problems such as (17) under strong regularity requirements on the right hand side $f$. In the present paper we focus on the first order formula under much lower regularity requirements, when applied to the fractional integral (1) and associated fractional diffusion equations.
3 Error analysis in the non smooth case

From (6) and (9) we obtain that the error at time \( t_n \) is given by

\[
\mathcal{I}_n^\alpha[f](t_n) - \mathcal{I}_n^\alpha[f] = \frac{\sin(\pi\alpha)}{\pi} \int_0^\infty x^{-\alpha} e_n(x) \, dx, \tag{21}
\]

with

\[ e_n(x) = y(x, t_n) - y_n(x). \]

As it is usually done to analyze the error for ODE solvers, we notice that \( y(x, t) \) solves the recurrence

\[
\frac{y(x, t_n) - y(x, t_{n-1})}{\tau_n} = -xy(x, t_n) + f(t_n) + d_n(x),
\]

with \( d_n \) Euler’s remainder, this is,

\[
d_n(x) = \frac{y(x, t_n) - y(x, t_{n-1})}{\tau_n} - y_t(x, t_n), \quad n \geq 1. \tag{22}
\]

Then

\[
e_n(x) = \sum_{k=1}^n \tau_k d_k(x) \prod_{j=k}^n r(\tau_j x). \tag{23}
\]

For the special case of \( f(t) = t^\beta \), with \( \beta > -1 \), we can obtain explicit representations of (23). For this, we recall the definition of the Mittag-Leffler function, see for instance [4].

**Definition 4 (Mittag-Leffler function).** For \( \alpha > 0, \beta \in \mathbb{R} \), the two parameter Mittag-Leffler function \( E_{\alpha,\beta}(z) \) is defined by

\[
E_{\alpha,\beta}(z) = \sum_{l=0}^\infty \frac{z^l}{\Gamma(\alpha l + \beta)}, \quad z \in \mathbb{C}.
\]

In the next result we collect a few identities and properties that will be needed in the proof of Theorem 12.

**Lemma 5.** It holds:

1. If \( f(t) = t^\ell \), with \( \ell > -1 \),

\[
\mathcal{I}_n^\alpha[f](t) = \frac{\Gamma(\ell + 1)}{\Gamma(\alpha + \ell + 1)} t^{\alpha + \ell}. \tag{24}
\]

2. For \( \beta > -1, \beta \neq 0 \), the solution \( y(x, t) \) to (7) with \( f(t) = t^\beta \) satisfies

\[
y(x, t) = \Gamma(1 + \beta) t^{\beta+1} E_{1,\beta+2}(-xt), \tag{25}
\]

\[
y_t(x, t) = \Gamma(1 + \beta) t^{\beta} E_{1,\beta+1}(-xt), \tag{26}
\]

\[
y_{tt}(x, t) = \Gamma(1 + \beta) t^{\beta-1} E_{1,\beta}(-xt). \tag{27}
\]

For \( \beta = 0 \) (25) and (26) still hold true, but (27) must be replaced by

\[
y_{tt}(x, t) = -xe^{-xt}. \tag{28}
\]

3. From [20, Theorem 1.6], for \( \alpha < 2 \) and \( \beta \in \mathbb{R} \), there exists \( C > 0 \) such that

\[
|E_{\alpha,\beta}(-y)| \leq \frac{C}{1 + y}, \quad y \geq 0. \tag{29}
\]
Proof. Identity (24) follows directly by noticing that the Laplace transform of the left hand side is \( \Gamma(\ell + 1)z^{-\ell-\alpha-1} \).

In order to prove (25), we write
\[
y(x, t) = \int_0^t (t-s)\beta e^{-xs} \, ds = \Gamma(1 + \beta) \mathcal{L}^{1+\beta}[e^{-x}](t).
\]
By expanding the exponential into its power series and using the same argument as to prove (24), we can write
\[
y(x, t) = \sum_{\ell=0}^{\infty} \frac{(-x)^\ell}{\ell!} \int_0^t (t-s)^\beta \, ds
\]
\[
= \Gamma(1 + \beta) \sum_{\ell=0}^{\infty} \frac{(-x)^\ell}{\ell!} \frac{\Gamma(\ell + 1) t^{\beta+\ell+1}}{\Gamma(\ell + \beta + 2)}
\]
\[
= \Gamma(1 + \beta) t^{\beta+1} E_{1,\beta+2}(-xt),
\]
this is (25).
Derivation of the power series gives
\[
y_t(x, t) = \Gamma(1 + \beta) \sum_{\ell=0}^{\infty} \frac{(-x)^\ell}{\ell!} \frac{\Gamma(\ell + 1) t^{\beta+\ell+1}}{\Gamma(\ell + \beta + 1)}
\]
and so (26). The expression (27) for \( \beta \neq 0 \) follows analogously. For \( \beta = 0 \) the term in \( \ell = 0 \) is constant and thus we must use instead (28), which follows by differentiating twice in
\[
y(x, t) = \frac{1-e^{-xt}}{x}.
\] (30)

Lemma 6. Let \( \beta > -1 \), and \( f(t) = t^\beta \) in (7). Then
\[
d_1(x) = -\tau_1^\beta \Gamma(1 + \beta) (E_{1,\beta+1}(-x\tau_1) - E_{1,\beta+2}(-x\tau_1))
\] (31)
and, for \( k > 1 \), there exist \( \xi_k \in (t_{k-1}, t_k) \) such that
\[
d_k(x) = \begin{cases} 
-\frac{\tau_k}{2} \Gamma(1 + \beta) \xi_k^{\beta-1} E_{1,\beta}(-x\xi_k), & \text{if } \beta \neq 0, \\
-\frac{x\tau_k}{2} e^{-x\xi_k}, & \text{if } \beta = 0.
\end{cases}
\] (32)

Proof. For \( k = 1 \) the result follows from (25) and (26), since
\[
d_1(x) = \frac{y(x, t_1)}{\tau_1} - y_t(x, t_1)
\]
For \( k \geq 2 \), we apply (27) or (28), according to the value of \( \beta \), to
\[
d_k(x) = \frac{y(x, t_k) - y(x, t_{k-1})}{\tau_k} - y_t(x, t_k) = -\frac{\tau_k}{2} y_{tt}(x, \xi_k).
\]
Proposition 7. For \( f(t) = t^\beta \) with \( \beta > -1 \) and for an arbitrary sequence of time points \( 0 < t_1 < \cdots < t_n \) with step sizes \( \tau_k = t_k - t_{k-1}, \ k \geq 1 \), there are \( \xi_k \in (t_{k-1}, t_k) \), for \( k \geq 2 \), such that the error in (21) can be bounded by

\[
|I_\alpha^\alpha[f](t_n) - I_n^\alpha[f]| \leq C \left( \tau_1^{\alpha+\beta} + \sum_{k=2}^{n} \tau_k^{2\alpha+\beta-2} \right),
\]

with \( C \) depending on \( \alpha \) and \( \beta \).

In particular, for \( t_n \) in (4), \( 1 \leq n \leq N \), it holds

\[
|I_\alpha^\alpha[f](t_n) - I_n^\alpha[f]| \leq \begin{cases} 
CT^{\alpha+\beta} N^{-\gamma(\alpha+\beta)}, & \gamma(\alpha + \beta) < 1, \\
CT^{\alpha+\beta} N^{-1}(1 + \log(n)), & \gamma(\alpha + \beta) = 1, \\
CT^{\alpha+\beta} N^{-1} t_n^{\alpha+\beta-1/\gamma}, & \gamma(\alpha + \beta) > 1.
\end{cases}
\]

Proof. We write

\[
I_\alpha^\alpha[f](t_n) - I_n^\alpha[f] = \frac{\sin(\pi \alpha)}{\pi} \int_0^\infty x^{-\alpha} e_n(x) \, dx
\]

\[
= \frac{\sin(\pi \alpha)}{\pi} \sum_{k=1}^{n} \tau_k \int_0^\infty x^{-\alpha} \left( \prod_{j=k}^{n} r(\tau_j x) \right) d_k(x) \, dx
\]

Noticing that for \( x > 0 \) it is \( x^{-\alpha} > 0 \) and \( 0 < r(\tau_j x) \leq 1 \), we can bound

\[
|I_\alpha^\alpha[f](t_n) - I_n^\alpha[f]| \leq \frac{\sin(\pi \alpha)}{\pi} \sum_{k=1}^{n} \tau_k \int_0^\infty x^{-\alpha} |d_k(x)| \, dx,
\]

provided that the integrals above are convergent.

For \( k = 1 \) we use (31) and (29) to obtain

\[
\tau_1 \int_0^\infty x^{-\alpha} |d_1(x)| \, dx
\]

\[
\leq \tau_1^{\beta+1} \Gamma(1 + \beta) \int_0^\infty x^{-\alpha} \left( |E_1,\beta+1(-x\tau_1)| + |E_1,\beta+2(-x\tau_1)| \right) \, dx
\]

\[
\leq 2C\tau_1^{\beta+1} \Gamma(1 + \beta) \int_0^{\infty} x^{-\alpha} \frac{1}{1 + x\tau_1} \, dx
\]

\[
= 2C\tau_1^{\alpha+\beta} \Gamma(1 + \beta) \int_0^{\infty} u^{-\alpha} \frac{1}{1 + u} \, du
\]

\[
= 2C\tau_1^{\alpha+\beta} \Gamma(1 + \beta) B(1 - \alpha, \alpha),
\]

for \( B \) the beta function.

For \( k > 1 \) and \( \beta = 0 \) we have, by Lemma 6,

\[
\int_0^{\infty} x^{-\alpha} |d_k(x)| \, dx = \frac{\tau_k}{2} \int_0^{\infty} x^{1-\alpha} e^{-x\xi_k} \, dx
\]

\[
= \frac{\tau_k}{2} \xi_k^{\alpha-2} \int_0^{\infty} u^{1-\alpha} e^{-u} \, du
\]

\[
\leq \Gamma(2 - \alpha) \frac{\tau_k}{2} \xi_k^{\alpha-2},
\]

for \( \xi_k \in (t_{k-1}, t_k) \).
For $k > 1$ and $\beta \neq 0$, we use (32) and (29) to bound
\[
\int_0^\infty x^{-\alpha} |d_k(x)| \, dx = \frac{\Gamma(1+\beta)}{2} \tau_k \xi_k^{\beta-1} \int_0^\infty x^{-\alpha} |E_{1,\beta}(-x\xi_k)| \, dx \\
\leq C \frac{\Gamma(1+\beta)}{2} \tau_k \xi_k^{\beta-1} \int_0^\infty x^{-\alpha} \frac{1}{1+x\xi_k} \, dx \\
= C \frac{\Gamma(1+\beta)}{2} \tau_k \xi_k^{\alpha+\beta-2} \int_0^\infty u^{-\alpha} \frac{1}{1+u} \, du, \quad \xi_k \in (t_{k-1}, t_k).
\]
This proves the general estimate (33).

We now notice that for the graded mesh in (4) we have
\[
\tau_k \leq \gamma \tau_k^{1/\gamma}, \quad k \geq 1,
\]
and that for $\beta < 2 - \alpha$ we can bound $\xi_k^{\alpha+\beta-2} \leq t_{k-1}^{\alpha+\beta-2}$, for $k \geq 2$. Thus
\[
\sin(\pi \alpha) \sum_{k=2}^n \tau_k \int_0^\infty x^{-\alpha} |d_k(x)| \, dx \\
\leq C \gamma^2 \tau^\gamma \sum_{k=2}^n k^{2(\gamma-1)} (k-1)^{(\alpha+\beta-2)}.
\]
We bound
\[
k^{2(\gamma-1)} (k-1)^{-2\gamma} = \left(1 + \frac{1}{k-1}\right)^{2\gamma} k^{-2} \leq 4^{\gamma} k^{-2}
\]
and then
\[
\frac{\sin(\pi \alpha)}{\pi} \left| \sum_{k=2}^n \tau_k \int_0^\infty x^{-\alpha} d_k(x) \, dx \right| \leq C \gamma^2 4^\gamma \tau^\gamma \sum_{k=2}^n k^{\gamma(\alpha+\beta)-2},
\]
and the result follows. For $\beta \geq 2 - \alpha$ we use the bound $\xi_k^{\alpha+\beta-2} \leq t_{k-1}^{\alpha+\beta-2}$ and derive the same result without the constant $4^\gamma$. \hfill \Box

**Remark 8.** Note that for $\alpha + \beta > 1$, the error estimate (33) on the uniform mesh with step size $\tau$ can be written as
\[
|I^\alpha[f](t_n) - I_n^\alpha[f]| \leq C \tau^{\alpha+\beta} + \sum_{k=2}^n \tau^2 \xi_k^{\alpha+\beta-2} \\
\leq C \tau^{\alpha+\beta} + \sum_{k=2}^n \tau^2 \max \left(t_k^{\alpha+\beta-2}, t_{k-1}^{\alpha+\beta-2}\right) \\
\leq \frac{C}{\alpha + \beta - 1} \tau^{\alpha+\beta-1},
\]
which is in agreement with the result in [15, Theorem 5.2]. Moreover, for $\alpha + \beta = 1$, the error estimate (33) on the uniform mesh can bounded by
\[
|I^\alpha[f](t_n) - I_n^\alpha[f]| \leq C \tau \left(1 + \log(n)\right), \quad n \geq 1.
\]

We will need the following generalization of the previous result to deal with remainder terms in power series expansions of the right hand side.
Corollary 9. For \( \sigma \geq 0 \) fixed, \( f(t) = (t - \sigma)^\beta_+ \), with \( \beta > 1 \) and \( (y)_+ := \max(0, y) \), and for an arbitrary sequence of time points \( 0 < t_1 < \cdots < t_n \) with step sizes \( \tau_n = t_n - t_{n-1} \), \( n \geq 1 \), there are \( \xi_k \in (t_{k-1}, t_k) \), for \( k \geq 2 \), such that the error in (21) can be bounded by

\[
|\mathcal{I}^\alpha[f](t_n) - \mathcal{I}_{n}[f]| \leq C \left( \tau_1(1 - \sigma)^{\alpha+\beta-1} + \sum_{k=2}^{n} \tau_k^2(\xi_k - \sigma)^{\alpha+\beta-2} \right),
\]

with \( C \) depending on \( \alpha \) and \( \beta \).

Proof. We observe that

\[
y(x, t) = \begin{cases} 
0, & \text{if } t < \sigma \\
\mu(x, t - \sigma), & \text{if } t \geq \sigma,
\end{cases}
\]

where \( \mu \) is the solution to \( (7) \) with right hand side \( t^\beta \). The restriction to \( \beta > 1 \) guarantees that \( y(x, t) \) in \( (7) \) is twice differentiable with respect to \( t \) in \( (0, T) \), with \( y_t \) bounded, and obvious formulas follow for \( y_t \) and \( y_{tt} \). This leads to the following generalization of (31)

\[
d_1(x) = \frac{y(x, \tau_1)}{\tau_1} - \mu(x, \tau_1) = \Gamma(1 + \beta)(\tau_1 - \sigma)^\beta \left( \frac{\tau_1 - \sigma}{\tau_1} E_{1, \beta + 2}(-x(\tau_1 - \sigma)) - E_{1, \beta + 1}(-x(\tau_1 - \sigma)) \right)
\]

and of (32)

\[
d_k(x) = -\frac{\tau_k}{2} \Gamma(1 + \beta)(\xi_k - \sigma)^{\beta-1} E_{1, \beta}(-x(\xi_k - \sigma)).
\]

The integrals in the proof of Proposition 7 are then either 0 or can be estimated by the analogous expressions with \( \tau_1 \) or \( \xi_k \) shifted by \( \sigma \).

Denote the Riemann-Liouville fractional derivative of order \( \mu > 0 \) by

\[
f^{(\mu)}(t) = \frac{d^\mu}{dt^\mu} \mathcal{I}^{\rho - \mu}[f](t),
\]

with \( \mu > 0, \rho - 1 \leq \mu < \rho, \rho \in \mathbb{N} \), where \( \mathcal{I}^{\rho - \mu} \) is the fractional integral (1) of order \( \rho - \mu \). For \( \mu < 0 \) we take \( f^{(\mu)} = \mathcal{I}^{\mu} \).

Lemma 10. [20, (2.108)] Let \( \mu > 0 \), \( \rho - 1 \leq \mu < \rho, \rho \in \mathbb{N} \), if the fractional derivative \( f^{(\mu)}(t) \) is integrable, then

\[
\mathcal{I}^{\mu}[f^{(\mu)}](t) = f(t) - \sum_{t=1}^{\rho} \frac{f^{(\mu - \ell)}(0)}{\Gamma(\mu - \ell + 1)} t^{\mu - \ell}.
\]

According to the definition of the fractional integral (1), Lemma 10 gives the fractional Taylor expansion of \( f(t) \) at \( t = 0 \) with remainder in integral form, cf. [14, (3.20)]. Starting from this, we introduce the following proposition.

Proposition 11. Assume that \( \mu > 2 \), \( f^{(\mu - \ell)}(0) = 0 \), for \( \ell = 1, \ldots, \rho \), with \( \rho - 1 \leq \mu < \rho \), and \( f^{(\mu)} \) is integrable. Then, for an arbitrary sequence of time points \( 0 < t_1 < \cdots < t_n \) with step sizes \( \tau_n = t_n - t_{n-1} \), \( n \geq 1 \), there exist \( \xi_k \in (t_{k-1}, t_k) \), for \( k \geq 2 \), such that the following bound holds

\[
|\mathcal{I}^\alpha[f](t_n) - \mathcal{I}_{n}[f]| \leq C \left( \tau_1^{\alpha+\mu} \max_{0 \leq t \leq t_1} |f^{(\mu)}(t)| + \sum_{k=2}^{n} \tau_k^2 \xi_k^{\alpha+\mu-2} \max_{0 \leq t \leq t_k} |f^{(\mu)}(t)| \right),
\]

with \( C \) depending on \( \alpha \) and \( \mu \).
Proof. By Lemma 10, \( f \) is equal to

\[
f(t) = T^\mu[f^{(\mu)}](t) = \frac{1}{\Gamma(\mu)} \left( t^{\mu-1} * f^{(\mu)} \right)(t).
\]  

Then

\[
T^\alpha[f](t_n) = \frac{1}{\Gamma(\alpha)} \int_0^{t_n} (t_n - s)^{\alpha-1} \int_0^s \frac{(s - u)^{-\mu-1}}{\Gamma(\mu)} f^{(\mu)}(u) du \ ds
\]

\[
= \frac{1}{\Gamma(\alpha)} \int_0^{t_n} (t_n - s)^{\alpha-1} \int_0^{t_n} \frac{(s - u)^{-\mu-1}}{\Gamma(\mu)} f^{(\mu)}(u) du \ ds
\]

\[
\int_0^{t_n} \frac{f^{(\mu)}(u)}{\Gamma(\mu)} \frac{1}{\Gamma(\alpha)} \int_0^{t_n} (t_n - s)^{\alpha-1} (s - u)^{-\mu-1} \ ds du
\]

\[
= \int_0^{t_n} \frac{f^{(\mu)}(u)}{\Gamma(\mu)} T^\alpha[(-u)^{-\mu-1}](t_n) du
\]

and

\[
T^\alpha_n[f] = \sum_{k=1}^n \omega_{n,k} \int_0^{t_n} (t_k - u)^{-\mu-1} f^{(\mu)}(u) du
\]

\[
= \sum_{k=1}^n \omega_{n,k} \int_0^{t_n} (t_k - u)^{-\mu-1} f^{(\mu)}(u) du
\]

\[
\int_0^{t_n} \frac{f^{(\mu)}(u)}{\Gamma(\mu)} \sum_{k=1}^n \omega_{n,k}(t_k - u)^{-\mu-1} du.
\]

Then

\[
T^\alpha[f](t_n) - T^\alpha_n[f] = \int_0^{t_n} \frac{f^{(\mu)}(u)}{\Gamma(\mu)} \left( T^\alpha[(-u)^{-\mu-1}](t_n) - T^\alpha_n[(-u)^{-\mu-1}] \right) du.
\]

Since \( \mu - 1 > 1 \), we can apply Corollary 9 and bound

\[
|T^\alpha[f](t_n) - T^\alpha_n[f]|
\]

\[
\leq C \int_0^{t_n} \left| \frac{f^{(\mu)}(u)}{\Gamma(\mu)} \right| \left( \tau_1 (\tau_1 - u)^{\alpha+\mu-2} + \sum_{k=2}^n \tau_k^2 (\xi_k - u)^{\alpha+\mu-3} \right) du
\]

\[
= C \frac{\max_{0 \leq t \leq \tau_1} \left| f^{(\mu)}(t) \right|}{\Gamma(\mu)} \tau_1 \int_0^{\tau_1} (\tau_1 - u)^{\alpha+\mu-2} du
\]

\[
+ C \sum_{k=2}^n \frac{\max_{0 \leq t \leq \xi_k} \left| f^{(\mu)}(t) \right|}{\Gamma(\mu)} \tau_k^2 \int_0^{\xi_k} (\xi_k - u)^{\alpha+\mu-3} du
\]

\[
= C \frac{\max_{0 \leq t \leq \tau_1} \left| f^{(\mu)}(t) \right|}{\Gamma(\mu)(\alpha + \mu - 1)} \tau_1^{\alpha+\mu} + C \sum_{k=2}^n \frac{\max_{0 \leq t \leq \xi_k} \left| f^{(\mu)}(t) \right|}{\Gamma(\mu)(\alpha + \mu - 2)} \tau_k^{\alpha+\mu-2}.
\]

And the result follows. \( \square \)

Our previous results allow to deal with functions of the form \( f(t) = t^\beta g(t) \), with \( \beta > -1 \) and \( g \) sufficiently smooth, as in [14]. We state now the main result of the paper.
Theorem 12. Let $\beta > -1$ and assume that $f(t)$ admits an expansion in fractional powers of the form

$$f(t) = \sum_{\ell=0}^{p} \frac{f^{(\ell+\beta)}(0)}{\Gamma(\ell + \beta + 1)} t^{\ell+\beta} + \frac{1}{\Gamma(p + \beta + 1)} \left( t^{p+\beta} * f^{(p+\beta+1)} \right)(t),$$

with $p > 1 - \beta$, $p \in \mathbb{N}$. Assume that $f^{(p+\beta+1)}$ is continuous on $[0,T]$. Then

$$|\mathcal{I}^\alpha[f](t_n) - \mathcal{I}^\alpha_n[f]|$$

$$\leq C \sum_{\ell=0}^{p} \left( \tau_1^{\ell+\alpha+\beta} + \sum_{k=2}^{n} \tau_k^{\ell+\alpha+\beta-2} \right) f^{(\ell+\beta)}(0)$$

$$+ C \left( \tau_1^{p+\alpha+\beta+1} \max_{0 \leq t \leq t_1} |f^{(p+\beta+1)}(t)| + \sum_{k=2}^{n} \tau_k^{2(p+\alpha+\beta-1)} \max_{0 \leq t \leq t_k} |f^{(p+\beta+1)}(t)| \right),$$

for a general time mesh in (8), $\xi_k \in (t_{k-1}, t_k)$ with $k \geq 2$ and a constant $C$ depending on $\alpha$ and $\beta$.

For $\beta > 1 - \alpha$, the above error estimate is $O(\tau_{\text{max}})$, for any sequence of time points and $f$ continuous. For $-\alpha < \beta \leq 1 - \alpha$ the condition $f^{(\beta)}(0) = 0$ guarantees a bound like $O(\tau_{\text{max}})$ and for $-1 < \beta \leq -\alpha$, we need $f^{(\beta)}(0) = f^{(\beta+1)}(0) = 0$.

Notice that the above result improves significantly the regularity requirements of the result in [11]. Notice also that for a graded mesh, Proposition 7 shows how to choose the grading parameter $\gamma$ in order to achieve convergence of order one, according to the regularity and the number of vanishing fractional moments at 0 of $f$.

4 Application to fractional diffusion equations

We consider the application of the gCQ method to fractional diffusion equations of the form

$$\partial_t^\alpha u(t) + Au(t) = f(t), \quad t \in (0,T],$$

$$u(0) = u_0,$$  

(39)

where $A$ is an elliptic operator, $0 < \alpha < 1$, and $\partial_t^\alpha$ denotes the Caputo fractional derivative of order $\alpha$

$$\partial_t^\alpha u(t) := \mathcal{I}^{1-\alpha}[\partial_t u](t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} \frac{d}{ds} u(s) ds.$$

The Laplace transform of the solution is given by

$$U(z) = z^{\alpha-1}(z^\alpha I + A)^{-1} u_0 + (z^\alpha I + A)^{-1} F(z),$$

with $F(z)$ the Laplace transform of the source $f(t)$. By using the operational notation for convolutions in [15], see Remark 2, we can write the solution as

$$u(t) = E(t) u_0 + (K(\partial_t) f)(t),$$

(40)

with

$$E(t) = \mathcal{L}^{-1}[z^{\alpha-1}(z^\alpha I + A)^{-1}](t)$$

(41)

and

$$K(z) = (z^\alpha I + A)^{-1}.$$  

(42)

We denote further

$$k(t) = \mathcal{L}^{-1}[K](t),$$

(43)
which satisfies \((k \ast f)(t) = (K(\partial_t)f)(t)\).

Let us assume first that \(u_0 \in D(A)\). Then, we can use the identity
\[
(z^\alpha I + A)^{-1}z^\alpha = I - (z^\alpha I + A)^{-1}A
\]
to write
\[
E(t)u_0 = u_0 - K(\partial_t)Au_0. \tag{44}
\]
Combining (40) with (44) yields
\[
v(t) := u(t) - u_0 = (K(\partial_t)(f - Au_0))(t),
\]
which is the solution of
\[
\partial^\alpha_t v(t) + Av(t) = f(t) - Au_0, \quad t \in (0,T]. \tag{45}
\]

By using now the notation
\[
K(\partial_t^\alpha)f
\]
for the gCQ discretization of \(K(\partial_t)f\) on an arbitrary time grid \(\Delta := 0 < t_1 < \cdots < t_N = T\), we obtain for the smooth case \(u_0 \in D(A)\) at \(t_n\), the scheme
\[
\left( (\partial_t^\alpha)^n v \right)_{n+1} + Av_n = f(t_n) - Au_0, \quad n \geq 1, \tag{46}
\]
where \(\partial_t^\alpha\) denotes the approximation of the first order derivative provided by the gCQ method, this is,
\[
(\partial_t^\alpha v)_n = \frac{v_n - v_{n-1}}{\tau_n}, \quad 1 \leq n \leq N.
\]
Since the gCQ preserves the composition rule of the continuous convolution, this yields the same approximation to \(v\) as
\[
K(\partial_t^\alpha)(f - Au_0).
\]
It then follows that the approximation properties of this scheme depend on the behavior of \(K(z)\) and the regularity of \(f - Au_0\).

If \(-A\) is a sectorial operator and the sectorial angle \(\delta\) can be taken arbitrarily close to zero, such as the Laplacian operator, we can deduce a real integral representation for \(k\) with similar properties to the one we use to analyze the gCQ discretization of (5).

**Theorem 13.** Let us assume that for any \(\delta > 0\), there exists \(M(\delta) > 0\) such that
\[
\| (zI + A)^{-1}z^\alpha \| \leq M(\delta)|z|^{-\alpha}, \quad \text{for } |\arg z| < \pi - \delta. \tag{47}
\]
Then, for \(0 < \alpha < 1\), \(k(t)\) in (43) can be represented by
\[
k(t) = \frac{\sin(\pi\alpha)}{\pi} \int_0^\infty x^\alpha (x^\alpha e^{-i\alpha \pi I + A})^{-1} (x^\alpha e^{i\alpha \pi I + A})^{-1} e^{-xt} dx, \tag{48}
\]

Proof. By (47), for \(0 < \alpha < 1\) and \(M = M((1 - \alpha)\pi)\), we can bound
\[
\| (z^\alpha I + A)^{-1} \| \leq M|z|^{-\alpha}, \quad \text{for } |\arg z| < \pi.
\]
Then
\[
\lim_{z \to 0, |\arg z| < \pi} z(z^\alpha I + A)^{-1} = 0
\]
and
\[ \lim_{z \to \infty, |\arg z| < \pi} (z^\alpha I + A)^{-1} = 0, \]

with \((z^\alpha I + A)^{-1}\) being defined and continuous for \(\text{Im} \ z \geq 0\), and also for \(\text{Im} \ z \leq 0\). By [5, Theorem 10.7d] the real inversion formula for the Laplace transform holds and
\[ k(t) = \frac{1}{2\pi i} \int_0^\infty e^{-xt} \left( ((xe^{-i\pi})^\alpha I + A)^{-1} - ((xe^{i\pi})^\alpha I + A)^{-1} \right) \, dx. \]

Formula (48) now follows from the identity
\[ ((xe^{-i\pi})^\alpha I + A)^{-1} - ((xe^{i\pi})^\alpha I + A)^{-1} = ((xe^{i\pi})^\alpha - (xe^{-i\pi})^\alpha) ((xe^{-i\pi})^\alpha I + A)^{-1} ((xe^{i\pi})^\alpha I + A)^{-1}. \]

Theorem 13 allows the following representation
\[ (k * (f - Au_0))(t) = \int_0^\infty G(x)\tilde{y}(x, t) \, dx, \]
with
\[ G(x) = \frac{\sin(\pi \alpha)}{\pi} x^\alpha (x^\alpha e^{-i\alpha\pi} I + A)^{-1} (x^\alpha e^{i\alpha\pi} I + A)^{-1} \]
and
\[ \partial_t \tilde{y}(x, t) = -x\tilde{y}(x, t) + f(t) - Au_0, \quad \tilde{y}(x, 0) = 0, \]
which is similar to (6). The bound
\[ ||G(x)|| \leq Mx^{-\alpha}, \quad x \in (0, \infty), \]
guarantees that the same convergence results obtained in Section 3 hold in this case. In particular, we can apply Proposition 7 to choose an optimally graded time mesh, according to the regularity of the source term \(f\).

In the non smooth case \(u_0 \notin D(A)\), we can approximate the solution (40) to (39) by applying the numerical inversion of sectorial Laplace transforms to approximate the term \(E(t)u_0\) and the gCQ method to deal with the convolution \(K(\partial_t)f\), for which Theorem 13 remains useful.

## 5 Implementation

We apply different quadratures proposed in the literature for computing the weights in (11). First of all we split the summation into a local and a history term like
\[ \mathcal{I}_n^\alpha[f] = \sum_{k=1}^{n-n_0} \omega_{n,k}f_k + \sum_{k=\max(1, n-n_0+1)}^{n} \omega_{n,k}f_k = \mathcal{I}_n^{\text{his}} + \mathcal{I}_n^{\text{loc}}, \]

for a fixed moderate value of \(n_0\), which can be also equal to 1, in principle. For the local term \(\mathcal{I}_n^{\text{loc}}\) we use the following complex-contour integral representation
\[ \mathcal{I}_n^{\text{loc}} = \frac{1}{2\pi i} \int_C z^{-\alpha} \sum_{k=1+(n-n_0)+1}^{n} \tau_k \left( \prod_{j=k}^{n} \frac{1}{1 - \tau_j z} \right) f_k \, dz, \quad n \geq 1, \]
where \( C \) is a clockwise oriented, closed contour contained in \( \Re(z) > 0 \), which encloses all poles of the integrand, namely \( \tau_k^{-1} \), with \( k = 1 + (n - n_0)_+, \ldots, n \). We denote

\[
u_n^{\text{loc}}(z) := \sum_{k=1}^{n} \tau_k \left( \prod_{j=k}^{n} \frac{1}{1 - \tau_j z} \right) f_k, \quad n \geq 1,
\]

which satisfies the recursion

\[
u_n^{\text{loc}}(z) = \frac{1}{1 - \tau_n z} \nu_{n-1}^{\text{loc}}(z) + \frac{\tau_n}{1 - \tau_n z} f_n, \quad \nu_{(n-n_0)_+}^{\text{loc}}(x) = 0
\]

and write

\[
I_n^{\text{loc}} = \frac{1}{2\pi i} \int_C z^{-\alpha} \nu_n^{\text{loc}}(z) \, dz. 
\] (52)

For the approximation of (52) we set \( m \) the minimum pole of (52), \( M \) the maximum one, and

\[ q := M/m. \]

Then we choose \( C \) as the circle \( C_M \) of radius \( M \) centered at \( M + m/10 \). The parametrization of \( C_M \) and the quadrature nodes and weights for approximating (52) are obtained in the following way:

(i) If \( q < 1.1 \), we use the standard parametrization of \( C_M \) and apply the composite trapezoid rule. Notice that, in this case, the time grid \( \Delta \) is close to uniform and thus the special quadrature based on Jacobi elliptic functions from [12] is not required. The threshold value \( q = 1.1 \) has been found heuristically. In this case, the parametrization reads

\[
\tilde{\gamma}_M(\theta) = m/10 + M(1 + e^{i\theta}), \quad \theta \in (-\pi, \pi),
\]

and the quadrature nodes and weights are given by

\[
z_l = \tilde{\gamma}_M(\theta_l), \quad w_l = \frac{\tilde{\gamma}_M'(\theta_l)}{iN_Q^{\text{loc}}}, \quad \text{with} \quad \theta_l = -\pi + \frac{2\pi l}{N_Q^{\text{loc}}},
\] (53)

for \( l = 1, \cdots, N_Q^{\text{loc}} \).

(ii) If \( q \geq 1.1 \), we apply the quadrature proposed in [12] which is based on the special parameterization of \( C_M \)

\[
\tilde{\gamma}_M(\sigma) = m/10 + \frac{M}{q-1} \left( \sqrt{2q - 1} \frac{\lambda^{-1/2} + \text{sn}(\sigma, \lambda)}{\lambda^{-1/2} - \text{sn}(\sigma, \lambda)} - 1 \right),
\] (54)

where \( \text{sn} \) is the elliptic sine function. The quadrature nodes \( z_l \) and weights \( w_l \) in this case are given by

\[
z_l = \tilde{\gamma}_M(\sigma_l), \quad w_l = \frac{4K(\lambda)}{2\pi iN_Q^{\text{loc}}} \tilde{\gamma}_M'(\sigma_l),
\] (55)

for \( l = 1, \cdots, N_Q^{\text{loc}} \).

Notice that if we are solving an integral equation, such as in the application to (39), then \( f_n \) is not known at step \( t_n \). In this case, we can apply Cauchy Theorem and write

\[
I_n^{\text{loc}} \approx \tau_n^\alpha f_n + \sum_{l=1}^{N_Q^{\text{loc}}} w_l z_l^{-\alpha} \frac{1}{1 - \tau_n z_l} \nu_{n-1}^{\text{loc}}(z_l) =: \tilde{I}_n^{\text{loc}}.
\] (56)

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For the history term in (50) we adapt the quadrature proposed in [1] to deal with the variable time grid. We write
\[ I_n^{\text{his}} = \sum_{k=1}^{n-n_0} \omega_{n,k} f_k = \frac{\sin(\pi \alpha)}{\pi} \int_0^\infty x^{-\alpha} \left( \prod_{j=n-n_0+1}^{n} r(\tau_j x) \right) u_{n-n_0}^{\text{his}}(x) \, dx, \tag{57} \]
with \( r(x) \) defined in (12) and
\[ u_n^{\text{his}}(x) := \sum_{k=1}^{n} \tau_k \left( \prod_{j=k}^{n} \frac{1}{1 + \tau_j x} \right) f_k, \]
which satisfies the recursion
\[ u_j^{\text{his}}(x) = \frac{1}{1 + \tau_j x} u_{j-1}^{\text{his}}(x) + \frac{\tau_j}{1 + \tau_j x} f_j, \quad u_0^{\text{his}}(x) = 0. \tag{58} \]
Denote by \( N_Q^{\text{his}} \) the total number of quadrature nodes \( x_l \) and weights \( \omega_l \) in [1, Section 4], \( l = 1, \ldots, N_Q^{\text{his}} \). The integral (57) can then be approximated by
\[ I_n^{\text{his}} \approx \sum_{l=1}^{N_Q^{\text{his}}} \omega_l \left( \prod_{j=n-n_0+1}^{n} r(\tau_j x_l) \right) u_{n-n_0}^{\text{his}}(x_l) =: \tilde{I}_n^{\text{his}}. \tag{59} \]
Notice that due to the recursion (58), the evaluation of \( I_n^{\text{his}} \) for \( 1 \leq n \leq N \) requires a number of operations proportional to \( N \) and storage proportional to \( N_Q^{\text{his}} \). We finally approximate
\[ \mathcal{I}_n[f] \approx \tilde{I}_n^{\text{his}} + \tilde{I}_n^{\text{loc}}, \quad n \geq 1. \]
In our numerical experiments, we set
\[ n_0 = \min(10, N), \quad N_Q^{\text{loc}} = \max(50, n_0^2), \]
for the evaluation of \( \tilde{I}_n^{\text{loc}} \). In this way the total complexity of this algorithm is \( O(n_0 N_Q^{\text{loc}} + (N - n_0) N_Q^{\text{his}}) \), while the memory requirements grow like \( O(N_Q^{\text{loc}} + N_Q^{\text{his}}) \). For the uniform step approximation of (1), this is, the original CQ, we prove in [1] that \( N_Q^{\text{his}} = O(\log(N)) \). For a variable step implementation we also observe \( N_Q^{\text{his}} \ll N \), as shown in Tables 2-4. However we notice that the quadrature in [1] turns out to be inaccurate on very strongly graded meshes, with \( \gamma > 4 \). In this case we resorted to the quadrature from [12] globally, this is, \( \mathcal{I}_n[f] \approx \tilde{I}_n^{\text{loc}} \), for every \( n = 1, \ldots, N \) (corresponding to \( n_0 = N \)). This latter choice turned out to be more reliable for very strongly graded meshes but we lose in this case the fast and oblivious implementation for the history term.

6 Numerical experiments

We test in this Section the convergence results proven in Proposition 7 and Section 4, by applying the gCQ method to different examples. Since the main goal of this paper is to derive accurate error estimates for the gCQ rather than developing an optimal algorithm for its implementation, we set a rather high tolerance requirement of the quadratures described in the previous Section, for all values of the total number \( N \) of time steps. More precisely, we set \( \text{tol} = 10^{-12} \) for the evaluation of \( \tilde{I}_n^{\text{his}} \) by the quadrature in [1], which is modified to deal with a non uniform time grid. Essentially this generalization is accomplished by replacing the constant time step in the original CQ, for which the algorithm in [1] is designed, by the minimal time step if a non uniform time grid is chosen. The development of a more optimized algorithm is beyond the scope of the present paper.
6.1 Computation of the fractional integral

To verify Proposition 7, we consider the approximation to the fractional integral (1) with

\[ f(t) = t^\beta. \]

The exact solution is then given by

\[ I_\alpha[f](t) = \frac{\Gamma(\beta + 1)}{\Gamma(\alpha + \beta + 1)} t^{\alpha+\beta}. \]  

(60)

Set \( T = 1 \). The maximum absolute error is measured by

\[ \max_{1 \leq n \leq N} |I_\alpha[f](t_n) - I_n^\alpha[f]|. \]

For \( \alpha = 0.8 \) and \( \gamma = 1/(\alpha + \beta) \), the value of \( N^h_Q \) in (59) is listed in Table 1, which shows that the quadrature number \( N^h_Q \) will increase moderately with increasing \( N \) or decreasing \( \beta \).

In Figure 1, we present the maximum absolute error for different values of \( \alpha \) and \( \beta \). The numerical results demonstrate that the gCQ method (9) can achieve first order convergence with \( \gamma = 1/(\alpha + \beta) \), which is consistent with the theoretical results. Further, in Figure 2, we test the relation between the convergence order and the grading parameter. We can observe that the convergence order is min \( (1, \gamma(\alpha + \beta)) \), in agreement with Proposition 7. In addition, the evolution of the error on different graded meshes (4) is presented in Figure 3, which shows that the error near the origin is much smaller for the nonuniform mesh than for the uniform one.

| \( \beta \) | \( N^h_Q \) used to approximate (60) with \( \alpha = 0.8, \gamma = \frac{1}{\alpha+\beta} \) |
|---|---|---|---|---|---|---|---|
| \( N \) | 2 | 4 | 5 | 6 | 7 | 8 | 9 |
| 0 | 34 | 47 | 56 | 63 | 67 | 75 | 77 |
| -0.1 | 36 | 52 | 63 | 67 | 75 | 79 | 83 |
| -0.2 | 40 | 56 | 67 | 75 | 79 | 86 | 87 |
| -0.3 | 44 | 62 | 74 | 80 | 87 | 92 | 94 |
| -0.4 | 48 | 70 | 83 | 87 | 94 | 95 | 94 |

Table 1: Number of \( N^h_Q \) in (59) used to approximate (60) with \( \alpha = 0.8, \gamma = \frac{1}{\alpha+\beta} \).

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Fig. 1. Maximum absolute error in the approximation of (60) with \( \gamma = \frac{1}{\alpha+\beta} \).
6.2 Fractional diffusion equations with non smooth data

Example 1. We consider the fractional ordinary diffusion equation
\[ \partial_t^\alpha u(t) + u(t) = f(t), \quad u(0) = 0, \quad 0 < t \leq 1, \]
with an exact solution
\[ u(t) = t^\beta. \]

The corresponding source term is
\[ f(t) = \frac{\Gamma(\beta + 1)}{\Gamma(\beta - \alpha + 1)} t^{\beta - \alpha} + t^\beta. \]

For the graded mesh (4) with \( \gamma = \frac{1}{4} \), the value of \( N^{^h_{\text{his}}} \) used in the computation is presented in Table 2 and, in Figure 4, we show the maximum errors for different values of \( \alpha \) and \( \beta \). The results show convergence of the gCQ method with full order one and are in agreement with the analysis in Section 4. In Figure 5 we show the convergence rate of this method for different graded meshes and, in particular, for the uniform mesh, which is \( O(N^{-\beta}) \).
Table 2: Value of $N_Q^{hix}$ for Example 1 with $\alpha = 0.5, \gamma = \frac{1}{\beta}$.

| $\beta \backslash N$ | $2^4$ | $2^5$ | $2^6$ | $2^7$ | $2^8$ | $2^9$ | $2^{10}$ |
|---------------------|-------|-------|-------|-------|-------|-------|---------|
| 0.4                 | 53    | 76    | 92    | 100   | 107   | 113   | 115     |
| 0.5                 | 47    | 68    | 81    | 92    | 98    | 103   | 107     |
| 0.6                 | 43    | 61    | 72    | 81    | 88    | 93    | 98      |
| 0.7                 | 40    | 56    | 66    | 72    | 81    | 85    | 93      |
| 0.8                 | 36    | 51    | 61    | 67    | 72    | 80    | 85      |

Fig. 4. Maximum absolute errors for Example 1 with $\gamma = \frac{1}{\beta}$.

Fig. 5. Maximum absolute errors for Example 1 with different values of $\gamma$.

**Example 2.** We consider here the following subdiffusion equation on a 1D domain $\Omega = (-1, 1)$:

$$\begin{align*}
\partial_t^\alpha u - \Delta u &= f(x,t), \quad (x,t) \in \Omega \times (0,1], \\
u(x,0) &= \cos(\pi x/2), \quad x \in \Omega, \\
u(x,t) &= 0, \quad (x,t) \in \partial \Omega \times (0,1].
\end{align*}$$

(61)

The exact solution is given by

$$u(x,t) = (1 + t^\beta) \cos(\pi x/2),$$

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and the source term is

\[ f(x, t) = \left( \frac{\Gamma(\beta + 1)}{\Gamma(\beta - \alpha + 1)} t^{\beta - \alpha} + \frac{\pi^2 (1 + t^3)}{4} \right) \cos(\pi x/2). \]

Problem (61) fits the format in (39) with \( A = -\Delta \) and \( u_0(x) = \cos(\pi x/2) \). The domain of \(-\Delta\) is given by

\[ D(-\Delta) = H^1_0(\Omega) \cap H^2(\Omega) \quad (62) \]

and \( u_0(x) \in D(-\Delta) \). Then, as discussed in Section 4, we can solve the equivalent problem (45).

We first discretize (45) in space by applying the finite element method with piecewise linear basis functions and mesh-width \( \Delta x \). The resulting discrete Laplacian operator is well known to satisfy the hypotheses of Theorem 13. Then, according to the regularity of \( f - \Delta u(x, 0) \), the convergence order of the gCQ method is one on graded meshes (4) with \( \gamma \geq 1/2 \). In this way we compute the numerical solution \( v^N_{\Delta x} \) of (45), and so \( u^N_{\Delta x} = v^N_{\Delta x} + u(x, 0) \). In our experiment we measure the maximum \( L^2 \)-norm error, this is,

\[ \max_{1 \leq n \leq N} \| u(t_n) - u^N_{\Delta x} \|_{L^2}. \]

In Figure 6 we show the expected result for \( \gamma = \frac{1}{2} \), for different values of \( \beta \). We also show in Table 3 the number of quadrature nodes \( N_{\text{his}}^Q \) used to approximate (46). In Figure 7 we display the error profiles for \( \alpha = \beta = 0.5 \), for both the uniform mesh and the optimal graded one, with \( \gamma = 2 \). We can see that the gCQ method on the nonuniform mesh is more accurate near \( t = 0 \).

**Table 3:** Value of \( N_{\text{his}}^Q \) for Example 2 with \( \alpha = 0.6, \gamma = \frac{1}{\beta} \).

| \( \beta \) \| \beta \| \beta \| \beta \| \beta \| \beta \| \beta | N | 2^4 | 2^5 | 2^6 | 2^7 | 2^8 | 2^9 | 2^{10} |
|---|---|---|---|---|---|---|---|
| 0.4 | 55 | 80 | 93 | 104 | 110 | 116 | 120 |
| 0.5 | 47 | 70 | 81 | 93 | 99 | 105 | 110 |
| 0.6 | 44 | 63 | 72 | 81 | 89 | 96 | 99 |
| 0.7 | 39 | 56 | 66 | 73 | 81 | 88 | 93 |
| 0.8 | 37 | 52 | 61 | 70 | 73 | 81 | 86 |

**Fig. 6.** Maximum \( L^2 \) norm error for Example 2 with \( \gamma = \frac{1}{\beta}, \Delta x = \frac{1}{3000} \).
Example 3. In this last example we consider the same equation as in the previous one but with some $u_0(x) \notin D(A)$, namely

$$\begin{cases}
\partial_t^\alpha u - \Delta u = f(x, t), & (x, t) \in \Omega \times (0, 1], \\
u(x, 0) = 1, & x \in \Omega, \\
u(x, t) = 0, & (x, t) \in \partial \Omega \times (0, 1].
\end{cases}$$

in $\Omega = (-1, 1)$ and with

$$f(x, t) = \left( \frac{\Gamma(\beta + 1)}{\Gamma(\beta - \alpha + 1)} t^{\beta-\alpha} + \pi^2(1 + t^\beta)/4 \right) \cos(\pi x/2).$$

As before we apply the linear finite element for the discretization in space of the problem. Then we approximate in time (39) with $A$ the resulting discrete Laplacian.

We apply the inversion method of the Laplace transform in [10] for the approximation of the term $E(t)u_0$ in (40). This gives

$$\mathcal{L}^{-1}[z^{\alpha-1}(z^\alpha I + A)^{-1}u_0](t_n) \approx \sum_{l=-J}^{J} \omega_l(t_n)z_l(t_n)z_l^{\alpha-1}(t_n)(z_l^\alpha(t_n)I + A)^{-1}u_0,$$

where

$$\omega_l(t_n) = -\frac{h}{2\pi i} \varphi'(lh), \quad z_l(t_n) = \varphi(lh),$$

with

$$\varphi(s) = \mu(t_n)(1 - \sin(\sigma + is)), \quad h = \frac{a(\theta)}{J}, \quad \mu(t_n) = \frac{2\pi dJ(1 - \theta)}{t_n a(\theta)},$$

$$a(\theta) = \text{arccosh} \left( \frac{1}{(1 - \theta)\sin(\sigma)} \right), \quad \theta = 1 - \frac{1}{J}, \quad d \in (0, \frac{\pi}{2} - \sigma),$$

for $1 \leq n \leq N$, with $\sigma = \frac{\pi}{4}$, $d = \frac{\pi}{6}$ and $J = 50$. Notice that we use a high number of quadrature points per time point, which is certainly not necessary, since the method in [10] is able to approximate the inverse Laplace transform with the same quadrature uniformly on time windows of the form $[t_0, \Lambda t_0]$, with $\Lambda \gg 1$. In this way we are approximating the term $E(t)u_0$ with machine precision and observe only the error induced by the gCQ approximation of the convolution term in (40).
The error in this example is measured with respect to a reference solution computed with double the time points, this is
\[
\max_{1 < n < N} \| u^{\Delta_x}_n - \tilde{u}^{2n}_{\Delta_x} \|_{L^2},
\]
where \( \tilde{u}^{2n}_{\Delta_x} \) is the corresponding numerical solution on the finer time mesh
\[
t_n = \left( \frac{n}{(2N)} \right)^\gamma, \quad 0 \leq n \leq 2N.
\]
The optimal grading parameter in (4) for this example is \( \gamma = \max \left( \frac{1}{\alpha}, \frac{1}{\beta} \right) \). In Table 4, we report the value of \( N^\text{his}_Q \) used in the quadrature formula (59) corresponding to this example.

**Table 4**: Value of \( N^\text{his}_Q \) for Example 3 with \( \alpha = 0.8, \gamma = \max \left( \frac{1}{\alpha}, \frac{1}{\beta} \right) \).

| \( \beta \) \( N \) | 2\(^4\) | 2\(^5\) | 2\(^6\) | 2\(^7\) | 2\(^8\) | 2\(^9\) | 2\(^{10}\) |
|---|---|---|---|---|---|---|---|
| 0.4 | 55 | 80 | 96 | 106 | 117 | 121 | 129 |
| 0.5 | 50 | 70 | 82 | 93 | 101 | 109 | 117 |
| 0.6 | 44 | 62 | 73 | 82 | 92 | 99 | 104 |
| 0.7 | 39 | 56 | 66 | 75 | 82 | 89 | 96 |
| 0.8 | 37 | 52 | 62 | 70 | 76 | 81 | 88 |

Fig. 8. Maximum \( L^2 \) norm error for Example 3 with \( \gamma = \max \left( \frac{1}{\alpha}, \frac{1}{\beta} \right), \Delta_x = \frac{1}{3000} \).

Fig. 9. Maximum \( L^2 \) norm error for Example 3 with \( \Delta_x = \frac{1}{3000} \).
The results in Figure 8 confirm that FEM-gCQ scheme for (63) is convergent with full order one on the graded mesh (4), with $\gamma = \max\left(\frac{1}{\alpha}, \frac{1}{\beta}\right)$. Figure 9 shows for different values of $\gamma$ the convergence order of this method, which is equal to $\min\{1, \gamma\alpha, \gamma\beta\}$.

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