EXPONENTIAL CONVOLUTION QUADRATURE FOR NONLINEAR SUBDIFFUSION EQUATIONS WITH NONSMOOTH INITIAL DATA*

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Abstract. An exponential type of convolution quadrature is proposed as a time-stepping method for the nonlinear subdiffusion equation with bounded measurable initial data. The method combines contour integral representation of the solution, quadrature approximation of contour integrals, multi-step exponential integrators for ordinary differential equations, and locally refined stepsizes to resolve the initial singularity. The proposed k-step exponential convolution quadrature can have kth-order convergence for bounded measurable solutions of the nonlinear subdiffusion equation based on natural regularity of the solution with bounded measurable initial data.

Key words. subdiffusion equation, time-fractional, nonlinear, nonsmooth initial data, high order, convolution quadrature, exponential integrator, locally refined stepsizes

AMS subject classifications. 65M12, 65M60, 35K55, 35Q35

1. Introduction.

This article is concerned with the construction and analysis of high-order time-stepping methods for the nonlinear subdiffusion equation

$$\begin{cases} \partial_t^\alpha u - \Delta u = f(u) & \text{in } \Omega \times (0,T], \\ u = 0 & \text{on } \partial\Omega \times (0,T], \\ u(0) = u_0 & \text{in } \Omega, \end{cases} \tag{1.1}$$

in a bounded Lipschitz domain $\Omega \subset \mathbb{R}^d$, with $d \geq 1$, with a given smooth function $f : \mathbb{R} \to \mathbb{R}$ and possibly nonsmooth initial value u_0, where $\partial_t^\alpha u$ denotes the Caputo fractional time derivative of order $\alpha \in (0,1)$ in time [13, p. 91], defined by

$$\partial_t^\alpha u := \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} \frac{\mathrm{d}}{\mathrm{d}s} u(s)\,\mathrm{d}s, \tag{1.2}$$

with $\Gamma(z) = \int_0^\infty s^{z-1} e^{-s} \mathrm{d}s$ being the gamma function.

Subdiffusion equation in the form of (1.1) have generated much interest in developing stable and accurate numerical methods as well as rigorous numerical analysis, due to its excellent modelling capability for various anomalously slow transport processes. Correspondingly, many efficient time-stepping methods have been proposed for solving the subdiffusion equations, including piecewise polynomial interpolation methods (such as L1 and L2 schemes), discontinuous Galerkin methods (dG), and convolution quadrature (CQ).

If the solution of the subdiffusion equation is sufficiently smooth (which requires the initial value to be smooth and satisfying sufficiently many compatibility conditions), then the L1 and L2 schemes, dG and CQ can all have desired high-order accuracy in solving subdiffusion equations, depending on the degree of polynomials used for generating the methods; see [10, 18, 24, 32, 27]. In this case, the error analysis in these articles can also be extended to nonlinear subdiffusion problems by applying some fractional versions of discrete Gronwall's inequality; see [11, 16, 17].

If the initial data are in $H_0^1(\Omega) \cap H^2(\Omega)$, but do not satisfy additional compatibility conditions, then the solutions of subdiffusion equations often have weak singularity

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at $t = 0$, satisfying the following estimate:

$$\|\partial_t^m u\|_{L^2} \le C_m t^{\alpha-m} \quad \text{for } m \ge 0, \tag{1.3}$$

where C_m is some constant that may depend on m. In this case, the L1, L2 and dG methods can still achieve the desired order of convergence by using variable stepsizes locally refined at $t = 0$; see [14, 15, 27, 28, 31]. If the initial value is in $\dot H^3(\Omega)$ (a little smoother than $H_0^1(\Omega) \cap H^2(\Omega)$), then it is shown in [5] that the spectral method using the recently developed log-orthogonal functions can achieve arbitrarily high-order accuracy. Similarly as the smooth case, the error analysis in these articles can be extended to nonlinear subdiffusion equations by using some fractional versions of discrete Gronwall's inequality. As far as we know, the analysis of these methods for nonsmooth initial data in $L^2(\Omega)$ or $L^\infty(\Omega)$ still remains open.

For nonsmooth initial data in $L^2(\Omega)$ or $L^\infty(\Omega)$ (without any differentiability), the regularity result in (1.3) no longer holds and should be replaced by a weaker one (see [12]):

$$\|\partial_t^m u\|_{L^2} \le C_m t^{-m} \quad \text{for } m \ge 0. \tag{1.4}$$

In this case, the standard L1, L2, dG and CQ with uniform stepsizes generally have first-order convergence; see [9, 25, 10, 34]. The error analysis of L1, L2 and dG with variable stepsizes for nonsmooth initial data in $L^2(\Omega)$ or $L^\infty(\Omega)$ under the regularity condition (1.4) still remains open. For linear subdiffusion problems the $L1$, $L2$ and CQ methods with proper initial correction using a uniform stepsize can regain the desired high-order accuracy; see [10, 22, 34]. These methods, with initial corrections and uniform stepsize, typically have the following error bound for some $k \ge 1$:

$$\|u(t_n) - u_n\|_{L^2} \le C t_n^{-k} \tau^k \quad \text{for a uniform stepsize } \tau, \tag{1.5}$$

where C is some constant that is independent of the stepsize τ and t_n. It is also known that the algorithm in [3] based on Runge–Kutta CQ can have arbitrarily high-order accuracy for linear subdiffusion problems. For these methods, the high-order accuracy is achieved only when t_n is away from zero (when the initial data are nonsmooth), and the results do not hold for the nonlinear problem with nonsmooth initial data. The main difficulty of constructing high-order methods for a nonlinear subdiffusion problem with nonsmooth initial data is that the right-hand side $f(u)$ becomes singular at $t = 0$, and therefore the smoothness assumptions on the right-hand side in the above-mentioned articles are not fulfilled.

For the nonlinear subdiffusion problem (1.1), the backward Euler CQ can have first-order convergence for initial data with slight smoothness, i.e., $u_0 \in \dot H^s(\Omega)$ with $s > 0$; see [1]. However, high-order CQs generally can not achieve the optimal order of convergence. For example, high-order BDF CQs generally have at most $(1+2\alpha)$th-order convergence for initial data $u_0 \in H_0^1(\Omega) \cap C^2(\overline{\Omega})$, i.e.,

$$\|u(t_n) - u_n\|_{L^2} \le C t_n^{\alpha-s} \tau^s \quad \text{with } s = \min(k, 1 + 2\alpha - \epsilon), \tag{1.6}$$

where ϵ can be arbitrarily small. This order of convergence agrees with the numerical experiments, and was proved in [33] based on the regularity property

$$\|\partial_t^m u\|_{L^\infty} \le C_m t^{\alpha-m} \quad \text{for } m \ge 0, \tag{1.7}$$

which holds for initial value $u_0 \in H_0^1(\Omega) \cap C^2(\overline{\Omega})$. Therefore, there is an *order barrier* of high-order CQs for the nonlinear subdiffusion problem (due to the nonlinearity, in addition to the low regularity). This is very different from the linear problem. For nonsmooth initial data in $L^\infty(\Omega)$, the regularity result in (1.7) should be replaced by the following weaker result:

$$\|\partial_t^m u\|_{L^\infty} \le C_m t^{-m} \quad \text{for } m \ge 0. \tag{1.8}$$

Under this regularity, the construction and analysis of high-order time-stepping methods for the nonlinear subdiffusion problem still remain open, and will be addressed in this article in the L^∞ framework.

In this article, we propose a multistep exponential CQ for the nonlinear subdiffusion equation with initial data in $L^\infty(\Omega)$ based on contour integral representation of the solution and multistep exponential integrators for some ordinary differential equations appearing from the contour integral representation. The constructed k-step exponential CQ uses locally refined stepsizes towards $t = 0$ to resolve the singularity caused by nonsmooth initial data, and has the following properties that were not possessed by the CQs in literature:

1. kth-order convergence can be achieved for the nonlinear problem in (1.1) with nonsmooth initial data $u_0 \in L^\infty(\Omega)$, where k can be arbitrarily large.
2. Uniformly high-order accuracy can be achieved for all $t_n \in (0, T]$ for nonsmooth initial data in $L^\infty(\Omega)$, not necessarily away from $t = 0$.

The method proposed in this article generalizes multistep exponential integrators for nonlinear parabolic equations to nonlinear subdiffusion equations. The techniques developed here can also be applied for approximating general convolution operators by multistep exponential CQ.

The rest of this article is organized as follows. The construction of the time-stepping method is presented in Section 2 based on contour integral representation of the solution, quadrature approximation to the contour integrals, and a multistep exponential integrator with locally refined stepsizes. The main theorem on the convergence of the proposed method is presented at the end of Section 2. The proof of the main theorem is presented in Section 3. Numerical examples are presented in Section 4 to illustrate the accuracy of the proposed method for nonlinear subdiffusion problems with nonsmooth initial data. Some conclusions and remarks are presented in Section 5.

2. Construction of a multistep exponential CQ.

2.1. Notation and assumptions. We assume that $f : \mathbb{R} \to \mathbb{R}$ is a smooth function and therefore locally Lipschitz continuous, but not necessarily globally Lipschitz continuous. For example, $f(u) = u - u^3$ or $f(u) = e^u(1 - u^2)$ are smooth but not globally Lipschitz continuous with respect to u. Since $f(u)$ may not be integrable if u is unbounded, we require the initial value and solution to be bounded.

We say that u is a bounded mild solution of (1.1) if $u \in C([0, T]; L^2(\Omega)) \cap L^\infty(0, T; L^\infty(\Omega))$ and satisfies the following integral equation:

$$u(t) = u_0 + \Delta F(t)u_0 + \int_0^t E(t-s)f(u(s))\mathrm{d}s, \quad \forall\, t \in (0, T], \tag{2.1}$$

where $F(t)$ and $E(t)$ are the solution operators of the subdiffusion equation (see [11, (3.12)]), defined as the inverse Laplace transform of the operators $z^{-1}(z^\alpha - \Delta)^{-1}$ and $(z^\alpha - \Delta)^{-1}$, respectively, i.e.,

$$F(t) := \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\varphi,\delta}} e^{zt} z^{-1} (z^\alpha - \Delta)^{-1}\, \mathrm{d}z, \tag{2.2}$$

$$E(t) := \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\varphi,\delta}} e^{zt} (z^\alpha - \Delta)^{-1}\, \mathrm{d}z. \tag{2.3}$$

In the expressions (2.2)–(2.3), the integration is over the following contour on the complex plane (oriented with an increasing imaginary part):

$$\Gamma_{\varphi,\delta} = \Gamma^\delta_{\varphi,\delta} \cup \Gamma^\varphi_{\varphi,\delta} := \{z \in \mathbb{C} : |z| = \delta, |\arg z| \le \varphi\} \cup \{z \in \mathbb{C} : z = \rho e^{\pm \mathrm{i}\varphi}, \rho \ge \delta\}, \tag{2.4}$$

in which $\varphi \in (\frac{\pi}{2}, \pi)$ and $\delta > 0$ can be any fixed number. Since the integrand is analytic in z, the contour $\Gamma_{\varphi,\delta}$ can be deformed on the complement of the spectrum of the Dirichlet Laplacian operator.

It can be proved that the resolvent operator $(z-\Delta)^{-1} : L^\infty(\Omega) \to L^\infty(\Omega)$ satisfies the following estimate (a proof of this result can be found in Appendix):

$$\|(z-\Delta)^{-1}v\|_{L^\infty} \le C_\varphi |z|^{-1}\|v\|_{L^\infty} \quad \forall\, z \in \Sigma_\varphi,\ \ \varphi \in (\pi/2, \pi),\ \ \forall\, v \in L^\infty(\Omega), \tag{2.5}$$

where $\Sigma_\varphi = \{z \in \mathbb{C}\backslash\{0\} : |\arg(z)| \le \varphi\}$ is a sector on the complex plane.

Remark 2.1. If f is globally Lipschitz continuous, then the existence and uniqueness of a bounded mild solution satisfying (2.1) can be proved exactly as in [11, Proof of Theorem 3.1, Step 1] by using (A.3)–(A.4) and the Banach fixed-point argument (simply replacing X by $L^\infty(\Omega)$ in [11, Proof of Theorem 3.1, Step 1]). If f is not globally Lipschitz continuous but is the derivative of a double well potential, such as $f(u) = u - u^3$ (with two zeros at ± 1), then the maximum principle of time-fractional equations (see [35, Theorems 3.1–3.2] and [23, Theorem 2.1]) guarantees the existence and uniqueness of a bounded solution (e.g., $|u| \le 1$ for the solution of the nonlinear subdiffusion equation with $f(u) = u - u^3$).

In this article, we assume that the nonlinear subdiffusion problem (1.1) has a bounded mild solution and construct a high-order method for approximating the bounded mild solution. Throughout this article, we denote by $\varphi \in (\frac{\pi}{2}, \pi)$ a fixed angle, and denote by C a generic positive constant that may be different at different occurrences, but independent of $t_n \in [0, T]$ and the stepsize $\tau_n = t_n - t_{n-1}$.

2.2. Quadrature approximation of the solution. It is known that the Laplace transform in time of a function $g : [0, \infty) \to \mathbb{R}$ is defined as $\hat{g}(z) := \int_0^\infty e^{-zs} g(s)\mathrm{d}s$. The inverse Laplace transform has the following expression:

$$g(t) = \frac{1}{2\pi i}\int_{\mathrm{Re}(z)=\sigma} e^{zt}\hat{g}(z)\,\mathrm{d}z, \tag{2.6}$$

where σ is any positive number. If we denote $g(t) := f(u(t))$ and take the Laplace transform of (2.1) in time, then we obtain the following expression:

$$\hat{u}(z) = z^{\alpha-1}(z^\alpha - \Delta)^{-1}u_0 + (z^\alpha - \Delta)^{-1}\hat{g}(z) \quad \forall\, z \in \Sigma_\varphi. \tag{2.7}$$

By converting the expression back to the time variable through the inverse Laplace transform, we obtain

$$u(t) = \frac{1}{2\pi i}\int_{\mathrm{Re}(z)=\sigma} e^{zt}z^{\alpha-1}(z^\alpha - \Delta)^{-1}u_0\mathrm{d}z + \frac{1}{2\pi i}\int_{\mathrm{Re}(z)=\sigma} e^{zt}(z^\alpha - \Delta)^{-1}\hat{g}(z)\mathrm{d}z, \tag{2.8}$$

where σ is any positive number.

Since setting $g(s) = 0$ for $s \ge t$ does not affect the solution at time t, the above expression implies that

$$\begin{aligned} u(t) = &\frac{1}{2\pi i}\int_{\mathrm{Re}(z)=\sigma} e^{zt}z^{\alpha-1}(z^\alpha - \Delta)^{-1}u_0\mathrm{d}z \\ &+ \frac{1}{2\pi i}\int_{\mathrm{Re}(z)=\sigma} (z^\alpha - \Delta)^{-1}\int_0^t e^{z(t-s)}g(s)\mathrm{d}s\mathrm{d}z. \end{aligned} \tag{2.9}$$

This type of expressions for the solution avoids the use of $\hat{g}$ and was used in [20, 26]. In this paper we focus on the solution of (1.1) in a finite time interval $[0, T]$. Without loss of generality, we can extend $g(t) = f(u(t))$ to $t \in (T, \infty)$ with compact support without affecting the solution on $[0, T]$. For such extended $g(t)$ we can perform Laplace transform in (2.6) and derive the expression in (2.9) for $t \in [0, T]$, which actually does not depend on the extension of $g(t)$ to $t \in (T, \infty)$.

Since the integrand in (2.9) is analytic in z and has polynomial growth as $|z| \to \infty$ for $\mathrm{Re}(z) \le \sigma$, we can deform the contour of integration as in [11, 20], from the vertical line $\mathrm{Re}(z) = \sigma$ to the contour

$$\Gamma_\lambda = \{\lambda(1 - \sin(\beta + \mathrm{i}s)) : s \in \mathbb{R}\} \subset \Sigma_\varphi, \quad \text{with } \beta \in \Big(0, \varphi - \frac{\pi}{2}\Big), \tag{2.10}$$

where the parameter λ is to be determined later. As shown in Figure 2.1 (cf. [19, Figure 1]), the contour Γ_λ is intermediate between two sectors of angles $\beta + \frac{\pi}{2}$ and φ.

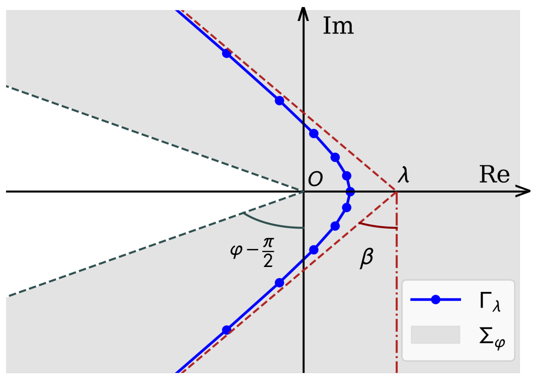

Fig. 2.1. *Location of the contour* Γ_λ *in* (2.10).

By substituting $g(s) = f(u(s))$ into the expression (2.9), we obtain

$$\begin{aligned} u(t) &= \frac{1}{2\pi i}\int_{\Gamma_\lambda} e^{zt} z^{\alpha-1}(z^\alpha - \Delta)^{-1} u_0 \mathrm{d}z + \frac{1}{2\pi i}\int_{\Gamma_\lambda} (z^\alpha - \Delta)^{-1} \int_0^t e^{z(t-s)} f(u(s)) \mathrm{d}s \mathrm{d}z \\ &= \frac{1}{2\pi i}\int_{\Gamma_\lambda} e^{zt} z^{\alpha-1}(z^\alpha - \Delta)^{-1} u_0 \mathrm{d}z + \frac{1}{2\pi i}\int_{\Gamma_\lambda} (z^\alpha - \Delta)^{-1} y(z,t) \mathrm{d}z, \end{aligned} \tag{2.11}$$

where

$$y(z,t) := \int_0^t e^{z(t-s)} f(u(s)) \mathrm{d}s. \tag{2.12}$$

In [19, Theorem 2.1] it is shown that the first integral in (2.11) can be approximated by a quadrature, i.e.,

$$\frac{1}{2\pi i}\int_{\Gamma_\lambda} e^{tz} z^{\alpha-1}(z^\alpha - \Delta)^{-1} u_0 \mathrm{d}z = \sum_{j=-M}^{M} w_j(t) e^{t z_j(t)} z_j^{\alpha-1}(t)(z_j^\alpha(t) - \Delta)^{-1} u_0 + \mathcal{E}_{1,q}(t), \tag{2.13}$$

where quadrature weights and quadrature nodes are given by

$$w_j(t) = -\frac{h}{2\pi i}\zeta'(jh) \;\text{ and }\; z_j(t) = \zeta(jh), \;\text{ with }\; \zeta(s) = \lambda(t)(1 - \sin(\beta + \mathrm{i}s)) \;\text{ for }\; s \in \mathbb{R}, \tag{2.14}$$

with

$$\begin{aligned} &h = \frac{a(\theta)}{M}, \quad \lambda(t) = \frac{2\pi d M(1-\theta)}{t\, a(\theta)} \\ &a(\theta) = \operatorname{arccosh}\left(\frac{\Lambda}{(1-\theta)\sin(\beta)}\right), \quad \theta = 1 - \frac{1}{M} \quad \text{and} \quad d \in (0, \frac{\pi}{2} - \beta). \end{aligned}$$

In [19, Theorem 2.1] it is shown that the above quadrature has exponential convergence with respect to M (the number of quadrature nodes), i.e.,

$$\|\mathcal{E}_{1,q}(t)\|_{L^\infty} \le C e^{-M/C}. \tag{2.15}$$

The second integral on the right-hand side of (2.11) can also be approximated by a quadrature:

$$\frac{1}{2\pi i}\int_{\Gamma_\lambda}(z^\alpha-\Delta)^{-1}y(z,t)\mathrm{d}z=\sum_{j=-M}^{M}\tilde{w}_j(\tilde{z}_j^\alpha-\Delta)^{-1}y(\tilde{z}_j,t)+\mathcal{E}_{2,q}(t), \tag{2.16}$$

with weights and nodes given by

$$\tilde{w}_j=-\frac{\tilde{h}}{2\pi i}\tilde{\zeta}'(j\tilde{h}),\quad \tilde{z}_j=\tilde{\zeta}(j\tilde{h}),\quad \tilde{h}=\sqrt{\frac{2\pi d}{\alpha M}}, \tag{2.17}$$

where $\tilde{\zeta}(s)=\tilde{\lambda}(1-\sin(\beta+\mathrm{i}s))$ and $\tilde{\lambda}$ is any fixed positive number. In Lemma 3.3 we prove the following error bound for the remainder in (2.16):

$$\|\mathcal{E}_{2,q}(t)\|_{L^\infty}\le Ce^{-\sqrt{2\pi d\alpha M}}. \tag{2.18}$$

Then, substituting (2.13) and (2.16) into (2.11), we obtain the following quadrature approximation of the solution:

$$\begin{aligned}u(t)=&\sum_{j=-M}^{M}w_j(t)e^{tz_j(t)}z_j^{\alpha-1}(t)(z_j^\alpha(t)-\Delta)^{-1}u_0+\sum_{j=-M}^{M}\tilde{w}_j(\tilde{z}_j^\alpha-\Delta)^{-1}y(\tilde{z}_j,t)\\&+\mathcal{E}_{1,q}(t)+\mathcal{E}_{2,q}(t).\end{aligned} \tag{2.19}$$

In the next subsection, we propose a parallel multistep exponential integrator for computing $y(\tilde{z}_j,t_n)$ from the past values $u(t_{n-j})$, $j=1,\dots,k$. Then the computed values of $y(\tilde{z}_j,t_n)$ can be substituted into (2.19) to yield the solution $u(t_n)$. This would yield a multistep method for the subdiffusion equation.

Remark 2.2. In [7], the solution of linear parabolic equation $\partial_t u(t)+Au(t)=f(t)$, with initial condition $u(0)=u_0$, is represented by

$$\begin{aligned}u(t)=&\frac{1}{2\pi i}\int_{\Gamma_I}e^{-zt}\left[(zI-A)^{-1}-\frac{1}{z}I\right]u_0\mathrm{d}z\\&+\int_0^t\frac{1}{2\pi i}\int_{\Gamma_I}e^{-z(t-s)}\left[(zI-A)^{-1}-\frac{1}{z}I\right]f(s)\mathrm{d}z\mathrm{d}s,\end{aligned}$$

where Γ_I is some hyperbola contour on the complex plane. The two contour integrals are discretized in [7] by quadratures, which are shown to have exponential convergence $O(e^{-c\sqrt{M}})$ under the condition that $f(t)\in D(A^\alpha)$ has an analytic extension $f(z)$ to a sector. The nonlinear subdiffusion problem considered in the current article differs from [7] significantly in that $f(u)$ depends nonlinearly on u (instead of t). Therefore, $f(u)$ is singular at $t=0$ and does not satisfy the conditions in [7].

2.3. The time-stepping method. Let k be any fixed positive integer, and let $\gamma\in(1-\frac{1}{k},1)$ be a given constant. We consider a partition $0=t_0<t_1<\cdots<t_N=T$ of the time interval $[0,T]$ with stepsize

$$\tau_1=\tau_2=T\Big(\frac{\tau}{T}\Big)^{\frac{1}{1-\gamma}}\quad\text{and}\quad \tau_n=t_n-t_{n-1}\sim\Big(\frac{t_{n-1}}{T}\Big)^\gamma\tau\quad\text{for } n\ge 3, \tag{2.20}$$

where τ is the maximal stepsize, and '$\sim$' means equivalent magnitude (up to a constant multiple). The stepsizes defined in this way have the following properties:

1. $\tau_n\sim\tau_{n-1}$ for two consecutive stepsizes.
2. $\tau_1\sim\tau^{\frac{1}{1-\gamma}}$, and $\tau_n=O(\tau^{\frac{1}{1-\gamma}})=O(\tau^k)$ for the starting time levels with $n=1,\dots,k-1$. Hence, the starting stepsize is much smaller than the maximal stepsize. This can resolve the solution's singularity at $t=0$.
3. The total number of time levels is $O(T/\tau)$. Hence, the total computational cost is equivalent to using a uniform stepsize τ.

From the definition of $y(z,t)$ in (2.12), it is straightforward to verify that $y(z,t)$

satisfies the following ordinary differential equation:

$$\partial_t y(z,t) = zy(z,t) + f(u(t)). \tag{2.21}$$

By the Duhamel formula of ordinary differential equations, the function $y(z,t)$ has the following expression:

$$y(z,t_n) = e^{z\tau_n} y(z,t_{n-1}) + \int_{t_{n-1}}^{t_n} e^{z(t_n-s)} f(u(s))\mathrm{d}s. \tag{2.22}$$

In this expression we further approximate $f(u(s))$ by its k-step extrapolation

$$f(u(s)) = \sum_{i=1}^{k} L_{ni}(s) f(u(t_{n-i})) + \mathcal{E}_f^n(s) =: I_\tau f(u)(s) + \mathcal{E}_f^n(s) \quad \text{for } s \in (t_{n-1}, t_n] \text{ and } n \ge k,$$

where $L_{ni}(s)$ is the unique polynomial of degree $k-1$ such that

$$L_{ni}(t_{n-j}) = \delta_{ij}, \quad j = 1, 2, \ldots, k.$$

Then we obtain

$$\begin{aligned} y(z,t_n) =& e^{z\tau_n} y(z,t_{n-1}) + e^{zt_n} \sum_{i=1}^{k} \left(\int_{t_{n-1}}^{t_n} e^{-zs} L_{ni}(s)\mathrm{d}s \right) f(u(t_{n-i})) \\ &+ \int_{t_{n-1}}^{t_n} e^{z(t_n-s)} \mathcal{E}_f^n(s)\mathrm{d}s. \end{aligned} \tag{2.23}$$

In view of (2.19) and (2.23), we propose the following time-stepping method for the semilinear subdiffusion equation (1.1): For $n \ge k$ we define

$$y_n(z) = e^{z\tau_n} y_{n-1}(z) + \sum_{i=1}^{k} \left(\int_{t_{n-1}}^{t_n} e^{z(t_n-s)} L_{ni}(s)\mathrm{d}s \right) f(u_{n-i}) \quad \text{at } z = \tilde{z}_j, \tag{2.24}$$

$$u_n = \sum_{j=-M}^{M} w_j(t_n) e^{z_j(t_n)t_n} z_j^{\alpha-1}(t_n)(z_j^\alpha(t_n) - \Delta)^{-1} u_0 + \sum_{j=-M}^{M} \tilde{w}_j (\tilde{z}_j^\alpha - \Delta)^{-1} y_n(\tilde{z}_j). \tag{2.25}$$

For $n = 1, \ldots, k-1$, we define

$$y_n(z) = e^{z\tau_n} y_{n-1}(z) + \int_{t_{n-1}}^{t_n} e^{z(t_n-s)} f(u_{n-1})\mathrm{d}s \quad \text{at } z = \tilde{z}_j, \tag{2.26}$$

$$u_n = \sum_{j=-M}^{M} w_j(t_n) e^{z_j(t_n)t_n} z_j^{\alpha-1}(t_n)(z_j^\alpha(t_n) - \Delta)^{-1} u_0 + \sum_{j=-M}^{M} \tilde{w}_j (\tilde{z}_j^\alpha - \Delta)^{-1} y_n(\tilde{z}_j). \tag{2.27}$$

Since $\tau_n = O(\tau^k)$ for $n = 1, \ldots, k-1$, the exponential Euler scheme in (2.26)–(2.27) can keep the errors of the numerical solution within $O(\tau^k)$ at the starting $k-1$ time levels.

Remark 2.3. It is known that the CQs generated by multistep methods and Runge–Kutta methods are equivalent to approximating the function $y(z,t)$ in (2.11) by solving (2.21) with the corresponding multistep methods and Runge–Kutta methods. In this article, we approximate the function $y(z,t)$ in (2.11) by solving (2.21) with a multistep exponential integrator with variable stepsizes, locally refined at $t = 0$ to resolve the singularity caused by nonsmooth initial data. Hence, the proposed method can be regarded as an exponential type CQ. In [21, equation (2.7)], the following method is used to approximate $y(t_{n+1})$:

$$y_{n+1} = e^{\tau_n \lambda} y_n + h \int_0^1 e^{(1-\theta)\tau_n \lambda} \left(\theta g(t_{n+1}) + (1-\theta) g(t_n)\right) d\theta,$$

which is the exponential integrator obtained by approximating $g(t)$ with its linear interpolation on $[t_n, t_{n+1}]$. The function $g(t)$ is assumed to be smooth in [21].

The main theoretical results of this article are presented in the following theorem.

Theorem 2.1. *Let $f : \mathbb{R} \to \mathbb{R}$ be a smooth function and $u_0 \in L^\infty(\Omega)$, and let the parameter γ in the stepsize choice* (2.20) *satisfy $1 - \frac{1}{k} < \gamma < 1$. If $u \in C([0,T]; L^2(\Omega)) \cap L^\infty(0,T; L^\infty(\Omega))$ is a bounded mild solution of* (1.1) *satisfying* (2.1)*, then there exists a positive constant τ_* such that when $\tau \le \tau_*$ the numerical solution given by the method* (2.24)–(2.27) *has the following error bound:*

$$\|u(t_n) - u_n\|_{L^\infty} \le C t_n^{\alpha-1}\tau^k + Ce^{-M/C} + Ce^{-\sqrt{2\pi d\alpha M}} \quad \text{for } n = 1, \dots, N. \tag{2.28}$$

If the parameter γ satisfies $1 - \frac{\alpha}{k} \le \gamma < 1$, then the error bound can be improved to

$$\|u(t_n) - u_n\|_{L^\infty} \le C\tau^k + Ce^{-M/C} + Ce^{-\sqrt{2\pi d\alpha M}} \quad \text{for } n = 1, \dots, N. \tag{2.29}$$

Remark 2.4. The error bound (2.28) only requires choosing a parameter $\gamma \in (1-\frac{1}{k}, 1)$ independent of $\alpha \in (0,1)$. The uniform error bound (2.29) requires choosing a parameter $\gamma \in (1 - \frac{\alpha}{k}, 1)$ depending on $\alpha \in (0,1)$.

Remark 2.5. From Theorem 2.1 we see that the numerical solution can have an error bound of $O(\tau^k)$ when

$$M \ge \frac{k^2}{2\pi d\alpha} |\ln(1/\tau)|^2.$$

The quadrature in (2.27) requires solving $2M + 1$ elliptic equations at every time level. For real-valued u_0 and f, it suffices to solve for $M + 1$ elliptic equations at every time level based on the relation $w_{-j}(t) = \overline{w_j(t)}$ and $\tilde{w}_{-j} = \overline{\tilde{w}_j}$. Since there are $O(\tau^{-1})$ time levels in total for computing the numerical solutions in $[0,T]$, the total computational cost would be $O(\tau^{-1}|\ln(1/\tau)|^2)$ for an error bound of $O(\tau^k)$ in the $L^\infty(\Omega)$ norm. Hence, the numerical methods has almost kth-order convergence (up to a logarithmic factor) for nonsmooth initial data in $L^\infty(\Omega)$.

3. Proof of Theorem 2.1.

In this section, we prove the error bound (2.28) for the proposed time-stepping method in (2.26)–(2.27). The error analysis is divided into two parts, i.e., the regularity analysis of a bounded mild solution and the error estimation that combines the stability and consistency analysis. The two parts are presented in the following two subsections, respectively.

3.1. Regularity of a bounded mild solution.

This section is devoted to a regularity at positive time for the nonlinear problem (1.1) if the source function f is smooth. The following estimates of the solution operators $F(t)$ and $E(t)$ defined in (2.2)–(2.3) are crucial in proving the regularity of solutions.

Lemma 3.1. *Let $\widetilde{F}(t) = I + \Delta F(t)$, where $F(t)$ is defined in* (2.2)*. Then the following estimates hold:*

$$\|\partial_t^j \widetilde{F}(t)\|_{L^\infty \to L^\infty} \le Ct^{-j} \quad \text{and} \quad \|\partial_t^j E(t)\|_{L^\infty \to L^\infty} \le Ct^{\alpha-1-j} \quad \text{for } j \ge 0. \tag{3.1}$$

Proof. By using the expression of the solution operators in (2.2), we find that

$$\begin{aligned}
\Delta F(t) &= \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\varphi,\delta}} e^{zt} z^{-1} \Delta (z^\alpha - \Delta)^{-1} \, \mathrm{d}z \\
&= -\frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\varphi,\delta}} e^{zt} z^{-1} \, \mathrm{d}z + \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\varphi,\delta}} e^{zt} z^{\alpha-1} (z^\alpha - \Delta)^{-1} \, \mathrm{d}z \\
&= -I + \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\varphi,\delta}} e^{zt} z^{\alpha-1} (z^\alpha - \Delta)^{-1} \, \mathrm{d}z,
\end{aligned}$$

where we have used the Cauchy integral formula to derive $\frac{1}{2\pi \mathrm{i}}\int_{\Gamma_{\varphi,\delta}} e^{zt}z^{-1}\,\mathrm{d}z = I$. This identity above implies that

$$\widetilde{F}(t) = \frac{1}{2\pi \mathrm{i}}\int_{\Gamma_{\varphi,\delta}} e^{zt}z^{\alpha-1}(z^\alpha-\Delta)^{-1}\,\mathrm{d}z.$$

Hence, by differentiating this expression in time, we obtain

$$\partial_t^j\widetilde{F}(t) = \frac{1}{2\pi \mathrm{i}}\int_{\Gamma_{\varphi,\delta}} e^{zt}z^{\alpha+j-1}(z^\alpha-\Delta)^{-1}\,\mathrm{d}z. \tag{3.2}$$

Then, using the resolvent estimate in (2.5), we have

$$\|(z^\alpha-\Delta)^{-1}v\|_{L^\infty} \le C_\varphi|z|^{-\alpha}\|v\|_{L^\infty} \quad \forall\, z\in\Sigma_\varphi,\ \ \forall\, v\in L^\infty(\Omega). \tag{3.3}$$

Substituting (3.3) into (3.2) yields that

$$\begin{aligned}
\|\partial_t^j\widetilde{F}(t)\|_{L^\infty\to L^\infty} &\le C\int_{\Gamma_{\varphi,\delta}} e^{\mathrm{Re}(z)t}|z|^{j-1}\,|\mathrm{d}z| \\
&= C\int_{\Gamma_{\varphi,\delta}^{\delta}} e^{\mathrm{Re}(z)t}|z|^{j-1}\,|\mathrm{d}z| + C\int_{\Gamma_{\varphi,\delta}^{\varphi}} e^{\mathrm{Re}(z)t}|z|^{j-1}\,|\mathrm{d}z| \\
&\le C\int_{-\varphi}^{\varphi} e^{\delta\cos(\theta)t}\delta^{j-1}\,\delta\mathrm{d}\theta + C\int_{\delta}^{\infty} e^{r\cos(\varphi)t}r^{j-1}\,\mathrm{d}r,
\end{aligned}$$

where we have decomposed the contour $\Gamma_{\varphi,\delta}$ into $\Gamma_{\varphi,\delta}^{\delta}\cup\Gamma_{\varphi,\delta}^{\varphi}$ as defined in (2.4). Note that $\varphi\in(\frac{\pi}{2},\pi)$ is fixed and therefore $\cos(\varphi)<0$, it follows that $e^{r\cos(\varphi)t} = e^{-|\cos(\varphi)|rt}$. In addition, since the parameter $\delta>0$ in the contour $\Gamma_{\varphi,\delta}$ of (3.2) can be arbitrary, choosing $\delta = t^{-1}$ yields

$$\begin{aligned}
\|\partial_t^j\widetilde{F}(t)\|_{L^\infty\to L^\infty} &\le C\int_{-\varphi}^{\varphi} e^{\cos(\theta)}t^{-j}\,\mathrm{d}\theta + C\int_{t^{-1}}^{\infty} e^{-|\cos(\varphi)|rt}r^{j-1}\,\mathrm{d}r \\
&\le C\int_{-\varphi}^{\varphi} t^{-j}\,\mathrm{d}\theta + Ct^{-j}\int_{1}^{\infty} e^{-|\cos(\varphi)|\rho}\rho^{j-1}\,\mathrm{d}\rho \\
&\le Ct^{-j}.
\end{aligned}$$

This proves the estimate for $\partial_t^j\widetilde{F}(t)$. The estimate for $\partial_t^jE(t)$ is similar and omitted. □

By using the estimates in Lemma 3.1 we can prove the following theorem on the regularity of bounded mild solutions.

Theorem 3.2. *If $f\in C^k(\mathbb{R})$ and $u\in C([0,T];L^2(\Omega))\cap L^\infty(0,T;L^\infty(\Omega))$ is a bounded mild solution of* (1.1)*, then*

$$\|\partial_t^k u(t)\|_{L^\infty} \le Ct^{-k} \quad \textit{for}\ \ t\in(0,T]. \tag{3.4}$$

Proof. The mean value theorem says that

$$|f(u)-f(v)| = \left|\left(\int_0^1 f'((1-\theta)v+\theta u)\mathrm{d}\theta\right)(u-v)\right| \le C\max_{|s|\le|u|+|v|}|f'(s)|\,|u-v|,$$

which implies that

$$\|f(u)-f(v)\|_{L^\infty} \le C\max_{|s|\le\|u\|_{L^\infty}+\|v\|_{L^\infty}}|f'(s)|\,\|u-v\|_{L^\infty}.$$

From the expressions

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}f(u(x,t)) = f'(u)\partial_t u, \\
&\frac{\mathrm{d}^2}{\mathrm{d}t^2}f(u(x,t)) = f''(u)(\partial_t u)^2 + f'(u)\partial_{tt}u,
\end{aligned}$$

we see that the time derivatives of $f(u)$ may have the following type of expressions:

$$\frac{\mathrm{d}^\ell}{\mathrm{d}t^\ell} f(u(t)) = \sum_{m_1+\cdots+m_j\le\ell} g_{m_1,\dots,m_j}(u)\partial_t^{m_1}u(t)\cdots\partial_t^{m_j}u(t) \quad \text{for } \ell\ge 1, \tag{3.5}$$

where $g_{m_1,\dots,m_j}(u)$ is some function of u and the summation extends over all possible positive integers $m_1,\cdots,m_j$ satisfying the constraint $m_1+\cdots+m_j\le\ell$. In fact, if (3.5) holds then differentiating it yields that it also holds for $\frac{\mathrm{d}^{\ell+1}}{\mathrm{d}t^{\ell+1}}f(u(t))$. Hence, by mathematical induction the expression (3.5) indeed holds for all $\ell\ge 1$. This expression implies the following inequality:

$$\begin{aligned}
&\left\|\frac{\mathrm{d}^\ell}{\mathrm{d}t^\ell} f(u(t))\right\|_{L^\infty} \qquad\qquad (3.6)\\
&\le C_{f,u,\ell}\sum_{j=1}^{\ell}\sum_{m_1+\cdots+m_j\le\ell}\|\partial_t^{m_1}u(t)\|_{L^\infty}\,\|\partial_t^{m_2}u(t)\|_{L^\infty}\,\cdots\,\|\partial_t^{m_j}u(t)\|_{L^\infty} \quad \text{for } \ell\ge 1,
\end{aligned}$$

where $C_{f,u,\ell}$ is a constant depending on f, $\|u\|_{L^\infty}$ and ℓ, and the inner summation extends over all possible positive integers $m_1,\cdots,m_j$ satisfying the constraint $m_1+\cdots+m_j\le\ell$. Since $u\in L^\infty(0,T;L^\infty(\Omega))$, the constant $C_{f,u,\ell}$ is bounded for $1\le\ell\le k$. Therefore we simply denote this constant by C.

By mathematical induction, we assume that for $m=0,\dots,\ell-1$, the following estimate holds (this is true for $\ell=1$):

$$\|\partial_t^m u(t)\|_{L^\infty}\le Ct^{-m}, \quad t\in(0,T]. \tag{3.7}$$

In the following, we prove that (3.7) also holds for $m=\ell$. In fact, substituting (3.7) into (3.6) yields

$$\left\|\frac{\mathrm{d}^m}{\mathrm{d}t^m} f(u(t))\right\|_{L^\infty}\le Ct^{-m}, \quad t\in(0,T], \quad \text{for } m=0,\dots,\ell-1. \tag{3.8}$$

By denoting $\widetilde{F}(t)=I+\Delta F(t)$ and multiplying (2.1) by t^ℓ, we obtain

$$\begin{aligned}
t^\ell u(t) &= t^\ell\widetilde{F}(t)u_0+\int_0^t (t-s+s)^\ell E(t-s)f(u(s))\mathrm{d}s\\
&= t^\ell\widetilde{F}(t)u_0+\sum_{j=0}^{\ell}\binom{\ell}{j}\int_0^t (t-s)^j E(t-s)s^{\ell-j}f(u(s))\mathrm{d}s\\
&=: t^\ell\widetilde{F}(t)u_0+\sum_{j=0}^{\ell}\binom{\ell}{j} w_{\ell,j}(t),
\end{aligned} \tag{3.9}$$

with

$$w_{\ell,j}(t)=\int_0^t g_j(t,s)\mathrm{d}s \quad \text{and} \quad g_j(t,s)=(t-s)^jE(t-s)s^{\ell-j}f(u(s)). \tag{3.10}$$

Since $g_j(t,s)$ contains a factor $(t-s)^j$, the time derivative up to jth-order would commute with the integral in (3.10). Therefore, differentiating (3.10) j times yields

$$\begin{aligned}
\partial_t^j w_{\ell,j}(t) &= \int_0^t \partial_t^j g_j(t,s)\,ds\\
&= \int_0^t \partial_t^j[(t-s)^jE(t-s)]s^{\ell-j}f(u(s))\mathrm{d}s\\
&= \int_0^t \partial_s^j\big[s^jE(s)\big](t-s)^{\ell-j}f(u(t-s))\,\mathrm{d}s \quad \text{(change of variable)}\\
&=: \int_0^t h_{\ell-j}(t,s)\,\mathrm{d}s.
\end{aligned} \tag{3.11}$$

Since the function $h_{\ell-j}(t,s) = \partial_s^j\big[s^j E(s)\big](t-s)^{\ell-j} f(u(t-s))$ contains a factor $(t-s)^{\ell-j}$, the time derivative up to $(\ell-j)$th-order would commute with the integral on the right-hand side of (3.11). Therefore, differentiating (3.11) $\ell - j$ times yields

$$\partial_t^{\ell-j}\partial_t^j w_{\ell,j}(t) = \partial_t^{\ell-j}\int_0^t h_{\ell-j}(t,s)\,ds = \int_0^t \partial_t^{\ell-j} h_{\ell-j}(t,s)\,ds,$$

which implies that

$$\partial_t^\ell w_{\ell,j}(t) = \int_0^t \partial_s^j(s^j E(s))\frac{\mathrm{d}^{\ell-j}}{\mathrm{d}t^{\ell-j}}[(t-s)^{\ell-j} f(u(t-s))]\mathrm{d}s, \quad \text{for } 0 \le j \le \ell.$$

As a result, we have

$$\begin{aligned}
\|\partial_t^\ell w_{\ell,j}(t)\|_{L^\infty} &\le \int_0^t C\|\partial_s^j(s^j E(s))\|_{L^\infty\to L^\infty}\left\|\frac{\mathrm{d}^{\ell-j}}{\mathrm{d}t^{\ell-j}}[(t-s)^{\ell-j} f(u(t-s))]\right\|_{L^\infty}\mathrm{d}s \\
&\le \int_0^t Cs^{\alpha-1}\left\|\frac{\mathrm{d}^{\ell-j}}{\mathrm{d}t^{\ell-j}}[(t-s)^{\ell-j} f(u(t-s))]\right\|_{L^\infty}\mathrm{d}s, \qquad (3.12)
\end{aligned}$$

where we have used the estimate $\|\partial_s^j(s^j E(s))\|_{L^\infty\to L^\infty} \le Cs^{\alpha-1}$, which is a consequence of the estimate in Lemma 3.1 and the product rule of differentiation.

If $1 \le j \le \ell$ then substituting (3.8) into (3.12) yields

$$\|\partial_t^\ell w_{\ell,j}(t)\|_{L^\infty} \le C, \quad 1 \le j \le \ell. \qquad (3.13)$$

If $j = 0$ then substituting (3.6) and (3.8) into (3.12) yields

$$\begin{aligned}
\|\partial_t^\ell w_{\ell,0}(t)\|_{L^\infty} &\le \int_0^t Cs^{\alpha-1}\left\|\frac{\mathrm{d}^\ell}{\mathrm{d}t^\ell}[(t-s)^\ell f(u(t-s))]\right\|_{L^\infty}\mathrm{d}s \\
&\le \int_0^t Cs^{\alpha-1}\sum_{j=1}^{\ell}\left\|[(t-s)^{\ell-j}\frac{\mathrm{d}^{\ell-j}}{\mathrm{d}t^{\ell-j}} f(u(t-s))]\right\|_{L^\infty}\mathrm{d}s \\
&\quad + \int_0^t Cs^{\alpha-1}\left\|[(t-s)^\ell\frac{\mathrm{d}^\ell}{\mathrm{d}t^\ell} f(u(t-s))]\right\|_{L^\infty}\mathrm{d}s \qquad \text{(product rule)} \\
&\le C + \int_0^t Cs^{\alpha-1}\left\|[(t-s)^\ell\frac{\mathrm{d}^\ell}{\mathrm{d}t^\ell} f(u(t-s))]\right\|_{L^\infty}\mathrm{d}s. \qquad (3.14)
\end{aligned}$$

By considering the cases $j \ge 2$ and $j = 1$ in (3.6), separately, we have

$$\begin{aligned}
&\left\|\frac{\mathrm{d}^\ell}{\mathrm{d}t^\ell} f(u(t-s))\right\|_{L^\infty} \le C\|\partial_t^\ell u(t-s)\|_{L^\infty} \\
&\quad + C\sum_{j=2}^{\ell}\sum_{m_1+\cdots+m_j\le\ell}\|\partial_t^{m_1}u(t-s)\|_{L^\infty}\,\|\partial_t^{m_2}u(t-s)\|_{L^\infty}\,\cdots\,\|\partial_t^{m_j}u(t-s)\|_{L^\infty} \\
&\qquad \le C(t-s)^{-\ell} + C\|\partial_t^\ell u(t-s)\|_{L^\infty}.
\end{aligned}$$

Substituting the inequality above into (3.14), we obtain

$$\begin{aligned}
\|\partial_t^\ell w_{\ell,0}(t)\|_{L^\infty} &\le C + \int_0^t Cs^{\alpha-1}\|(t-s)^\ell\partial_t^\ell u(t-s)\|_{L^\infty}\mathrm{d}s \\
&= C + \int_0^t C(t-s)^{\alpha-1}\|s^\ell\partial_s^\ell u(s)\|_{L^\infty}\mathrm{d}s, \qquad (3.15)
\end{aligned}$$

where we have made a change of variable in deriving the last equality. Now substituting (3.13) and (3.15) into (3.9) yields

$$\|\partial_t^\ell(t^\ell u(t))\|_{L^\infty} \le \|\partial_t^\ell(t^\ell\widetilde{F}(t)u_0)\|_{L^\infty} + \sum_{j=0}^{\ell}\binom{\ell}{j}\|\partial_t^\ell w_{\ell,j}(t)\|_{L^\infty}$$

$$\leq C + \int_0^t C(t-s)^{\alpha-1} \|s^\ell \partial_t^\ell u(s)\|_{L^\infty} \mathrm{d}s, \tag{3.16}$$

where we have used the first estimate in Lemma 3.1 in deriving the last inequality.

By using the product rule we can derive that

$$\|t^\ell \partial_t^\ell u(t)\|_{L^\infty} \leq \|\partial_t^\ell (t^\ell u(t))\|_{L^\infty} + C \sum_{j=1}^{\ell} \|t^{\ell-j} \partial_t^{\ell-j} u(t)\|_{L^\infty} \leq \|\partial_t^\ell (t^\ell u(t))\|_{L^\infty} + C,$$

where we have used the induction assumption (3.7) in the last inequality. The above inequality and (3.16) imply

$$\|t^\ell \partial_t^\ell u(t)\|_{L^\infty} \leq C + \int_0^t C(t-s)^{\alpha-1} \|s^\ell \partial_t^\ell u(s)\|_{L^\infty} \mathrm{d}s. \tag{3.17}$$

By using Gronwall's inequality, we derive

$$\|t^\ell \partial_t^\ell u(t)\|_{L^\infty} \leq C, \quad \forall\, t \in (0, T]. \tag{3.18}$$

This proves (3.7) for $m = \ell$, and therefore the mathematical induction is completed. $\square$

3.2. Error estimates. To this end, we first prove the error bound in (2.18) for the quadrature approximation in (2.16).

Lemma 3.3. *If $\|f(u)\|_{L^\infty(0,\,t;L^\infty)} \lesssim 1$, then the quadrature error bound* (2.18) *holds.*

Remark 3.1. The following proof only uses the boundedness of $\|f(u)\|_{L^\infty(0,\,t;L^\infty)}$, without using other properties of the function $f(u)$, hence the same quadrature error bound holds when we replace $f(u)$ by its extrapolation $\hat{I}_\tau f(u^{(\tau)})$.

Proof. If $\|f(u)\|_{L^\infty(0,\,t;L^\infty)} \lesssim 1$ then

$$\begin{aligned}
\|y(z,t)\|_{L^\infty} \leq \int_0^t e^{\mathrm{Re}(z)(t-s)} \|f(u(s))\|_{L^\infty} \mathrm{d}s &\lesssim \int_0^t e^{\mathrm{Re}(z)(t-s)} \mathrm{d}s \\
&= \frac{e^{\mathrm{Re}(z)t} - 1}{\mathrm{Re}(z)} \\
&\lesssim |z|^{-1} \quad \text{for } z \in \Gamma_\lambda,
\end{aligned}$$

and therefore

$$\|(z^\alpha - \Delta)^{-1} y(z,t)\|_{L^\infty} \lesssim |z|^{-1-\alpha} \quad \text{for } z \in \Gamma_\lambda. \tag{3.19}$$

If $s = x + iy$ then $\sin(\beta + is) = \sin(\beta - y)\cosh(x) + i\cos(\beta - y)\sinh(x)$, and therefore

$$\tilde{\zeta}(s) = \tilde{\lambda}(1 - \sin(\beta - y)\cosh(x)) - i\tilde{\lambda}\cos(\beta - y)\sinh(x).$$

By considering the asymptotic behaviour of $\tilde{\zeta}(x + iy)$ as $|x| \to \infty$, it is easy to verify that the function $\tilde{\zeta} : \mathbb{R} \to \mathbb{C}$ maps the strip

$$D_d = \{s \in \mathbb{C} : |\mathrm{Im}(s)| \leq d\}, \quad \text{with any fixed } d \in \Big(0, \frac{\pi}{2} - \beta\Big),$$

into some sector $\tilde{\lambda} + \Sigma_\phi$ for some $\phi \in (\frac{\pi}{2}, \pi)$. Since $|\zeta'(s)| \sim |\zeta(s)|$ as $|x| \to \infty$, the estimate in (3.19) implies that the function $g(s) = (\tilde{\zeta}(s)^\alpha - \Delta)^{-1} y(\tilde{\zeta}(s), t)\tilde{\zeta}'(s)$ decays exponentially as $x \to \pm\infty$, i.e., $|g(x + iy)| \lesssim e^{-\alpha|x|}$ for $x \in \mathbb{R}$ and $|y| \leq d$. Therefore, the function $g(s)$ satisfies the following conditions:

(i) $\int_{-d}^{d} |g(x + iy)| dy \to 0$ as $x \to \pm\infty$,
(ii) $\int_{\mathbb{R}} |g(x \pm id)| dx \lesssim 1$,
(iii) $|g(x)| \lesssim e^{-\alpha|x|}$ for $x \in \mathbb{R}$.

Under these conditions, it is shown in [30, Theorem 3.4] that the trapezoidal rule with mesh size $\tilde{h} = \sqrt{\frac{2\pi d}{\alpha M}}$ has the following exponential convergence:

$$\left| \int_{\mathbb{R}} g(x)\mathrm{d}x - \sum_{j=-M}^{M} g(j\tilde{h})\tilde{h} \right| \leq Ce^{-\sqrt{2\pi d\alpha M}}.$$

This proves the desired result. ∎

We denote by $u^{(\tau)}(s)$ the numerical solution which is piecewise linear in time and satisfies $u^{(\tau)}(t_n) = u_n$ for $n = 1, \ldots, N$. Denote $\hat{I}_\tau f(u^{(\tau)})$ be the extrapolation of $f(u)$ by using the values of the numerical solution $u^{(\tau)}$, i.e.,

$$\hat{I}_\tau f(u^{(\tau)})(s) = \begin{cases} \displaystyle\sum_{i=1}^{k} L_{ni}(s) f(u_{n-i}) & \text{for } s \in (t_{n-1}, t_n], \quad n \geq k, \\ f(u_{n-1}) & \text{for } s \in (t_{n-1}, t_n], \quad 1 \leq n \leq k-1. \end{cases}$$

Then we introduce an intermediate solution u_n^* defined by

$$y_n(z) = e^{z\tau_n} y_{n-1}(z) + \int_{t_{n-1}}^{t_n} e^{z(t_n - s)} \hat{I}_\tau f(u^{(\tau)})(s)\mathrm{d}s \quad \text{for } z \in \Gamma_\lambda, \tag{3.20}$$

$$u_n^* = \frac{1}{2\pi i} \int_{\Gamma_\lambda} e^{zt} z^{\alpha-1} (z^\alpha - \Delta)^{-1} u_0 \mathrm{d}z + \frac{1}{2\pi i} \int_{\Gamma_{\tilde{\lambda}}} (z^\alpha - \Delta)^{-1} y_n(z) \mathrm{d}z, \tag{3.21}$$

and consider the error decomposition

$$e_n = \tilde{e}_n + e_n^*, \quad \text{with} \quad \tilde{e}_n = u(t_n) - u_n^* \quad \text{and} \quad e_n^* = u_n^* - u_n. \tag{3.22}$$

We shall estimate $\tilde{e}_n$ and e_n^* separately.

To analyze the first part of the error, i.e., $\tilde{e}_n = u(t_n) - u_n^*$, we note that u_n^* coincides with the solution $u^*(t_n)$ of the semilinear diffusion equation

$$\begin{cases} \partial_t^\alpha u^* - \Delta u^* = \hat{I}_\tau f(u^{(\tau)}) & \text{in } \Omega \times (0, T], \\ u^* = 0 & \text{on } \partial\Omega \times (0, T], \\ u^*(0) = u_0 & \text{in } \Omega, \end{cases} \tag{3.23}$$

Meanwhile, we also note that the exact solution u satisfies the equation

$$\begin{cases} \partial_t^\alpha u - \Delta u = \hat{I}_\tau f(u) + \mathcal{E}_f & \text{in } \Omega \times (0, T], \\ u = 0 & \text{on } \partial\Omega \times (0, T], \\ u(0) = u_0 & \text{in } \Omega, \end{cases} \tag{3.24}$$

where the remainder $\mathcal{E}_f = f(u) - \hat{I}_\tau f(u)$ satisfies the following estimate for $t \in (t_{n-1}, t_n]$,

$$\|\mathcal{E}_f(t)\|_{L^\infty} \leq \begin{cases} C\tau_n^k \displaystyle\max_{s \in [t_{n-k}, t_n]} \left\| \frac{\mathrm{d}^k}{\mathrm{d}t^k} f(u(s)) \right\|_{L^\infty} \leq C\tau_n^k t_n^{-k} & \text{for} \quad n \geq k+1, \\ C \displaystyle\max_{s \in [0, t_k]} \|f(u(s))\|_{L^\infty} \leq C \leq C\tau_n^k t_n^{-k} & \text{for} \quad n = k, \\ C \displaystyle\max_{s \in [0, t_{k-1}]} \|f(u(s))\|_{L^\infty} \leq C = C\tau_1 t_1^{-1} & \text{for} \quad 1 \leq n \leq k-1, \end{cases} \tag{3.25}$$

where we have used Theorem 3.2 and (3.8), and the property $t_{n-k} \sim t_n$ for $n \geq k+1$ (as a result of the property $\tau_n \sim \tau_{n-1}$).

By using the expression (2.1) for the solution of the subdiffusion equation, the difference $\tilde{e} = u - u^*$ can be represented by

$$\tilde{e}(t_n) = \int_0^{t_n} E(t_n - s)(\hat{I}_\tau f(u) - \hat{I}_\tau f(u^{(\tau)}))\mathrm{d}s + \int_0^{t_n} E(t_n - s)\mathcal{E}_f(s)\mathrm{d}s \tag{3.26}$$

$$
\begin{aligned}
&= \left(\int_{t_{k-1}}^{t_n} E(t_n-s)(\hat{I}_\tau f(u) - \hat{I}_\tau f(u^{(\tau)}))\mathrm{d}s + \int_{t_{k-1}}^{t_n} E(t_n-s)\mathcal{E}_f(s)\mathrm{d}s \right) \\
&\quad + \left(\int_0^{t_{k-1}} E(t_n-s)(\hat{I}_\tau f(u) - \hat{I}_\tau f(u^{(\tau)}))\mathrm{d}s + \int_0^{t_{k-1}} E(t_n-s)\mathcal{E}_f(s)\mathrm{d}s \right) \\
&=: \widetilde{E}_{n,1} + \widetilde{E}_{n,2} \quad \text{for } \ n \geq k.
\end{aligned}
$$

By using the stepsize choice $\tau_j \sim \tau t_j^\gamma$, we have

$$
\begin{aligned}
\|\widetilde{E}_{n,1}\|_{L^\infty} &\leq C_{n,u^{(\tau)}} \sum_{j=k}^n \int_{t_{j-1}}^{t_j} (t_n-s)^{\alpha-1} \sum_{i=1}^k \|e_{j-i}\|_{L^\infty}\mathrm{d}s + C\sum_{j=k}^n \int_{t_{j-1}}^{t_j} (t_n-s)^{\alpha-1}\tau_j^k t_j^{-k}\mathrm{d}s \\
&\leq C_{n,u^{(\tau)}} \sum_{j=k}^n \tau_j (t_n - t_{j-1})^{\alpha-1} \sum_{i=1}^k \|e_{j-i}\|_{L^\infty} + C\tau^k \int_0^{t_n} (t_n-s)^{\alpha-1} s^{k(\gamma-1)}\mathrm{d}s \\
&\leq C_{n,u^{(\tau)}} \sum_{j=k}^n \tau_j (t_n - t_{j-1})^{\alpha-1} \sum_{i=1}^k \|e_{j-i}\|_{L^\infty} \\
&\quad + C\tau^k t_n^{\alpha+k(\gamma-1)} \qquad \text{when } \ k(\gamma-1) > -1,
\end{aligned} \tag{3.27}
$$

and

$$
\begin{aligned}
\|\widetilde{E}_{n,2}\|_{L^\infty} &\leq C_{n,u^{(\tau)}} \sum_{j=1}^{k-1} \int_{t_{j-1}}^{t_j} (t_n-s)^{\alpha-1} \|e_{j-1}\|_{L^\infty}\mathrm{d}s + C\sum_{j=1}^{k-1} \int_{t_{j-1}}^{t_j} (t_n-s)^{\alpha-1}\tau_j t_j^{-1}\mathrm{d}s \\
&\leq C_{n,u^{(\tau)}} \sum_{j=1}^{k-1} \tau_j (t_n - t_{j-1})^{\alpha-1} \|e_{j-1}\|_{L^\infty} + Ct_n^{\alpha-1} \sum_{j=1}^{k-1} \tau_j \\
&\leq C_{n,u^{(\tau)}} \sum_{j=1}^{k-1} \tau_j (t_n - t_{j-1})^{\alpha-1} \|e_{j-1}\|_{L^\infty} + Ct_n^{\alpha-1}\tau^k
\end{aligned} \tag{3.28}
$$

where $C_{n,u^{(\tau)}}$ is some positive constant which depends on $\|u_{j-1}\|_{L^\infty}$ for $j = 1, \ldots, n$, and the last inequality uses the property $\tau_j = O(\tau^k)$ for the starting $k-1$ time levels.

We use mathematical induction by assuming that the following inequality holds:

$$
\|e_j\|_{L^\infty} = \|u_j - u(t_j)\|_{L^\infty} \leq 1 \quad \text{for } \ 0 \leq j \leq m-1. \tag{3.29}
$$

Since $e_0 = 0$, this assumption holds for $m = 1$. Under this induction assumption, the constants $C_{n,u^{(\tau)}}$ in (3.27)–(3.28) are bounded for $1 \leq n \leq m$. Since the starting k steps are computed by the exponential Euler method with stepsize $\tau_n = O(\tau^k)$ for $n = 1, \ldots, k-1$, as a special case $k = 1$ of the analysis above, it follows that

$$
\begin{aligned}
\|\tilde{e}(t_n)\|_{L^\infty} \leq& C\sum_{j=1}^n \tau_j (t_n - t_{j-1})^{\alpha-1} \|e_{j-1}\|_{L^\infty} \\
&+ Ct_n^{\alpha-1}\tau^k \quad \text{when } \ k(\gamma-1) > -1, \quad n \geq 1.
\end{aligned} \tag{3.30}
$$

To analyze the second part of the error, i.e., $e_n^* = u_n^* - u_n$, we consider the difference between (3.21) and (2.27):

$$
\begin{aligned}
e_n^* &= \frac{1}{2\pi i}\int_{\Gamma_\lambda} e^{zt} z^{\alpha-1}(z^\alpha - \Delta)^{-1}u_0 \mathrm{d}z - \sum_{j=-M}^M w_j z_j^{\alpha-1}(t_n)(z_j^\alpha(t_n) - \Delta)^{-1}u_0 \\
&\quad + \frac{1}{2\pi i}\int_{\Gamma_\lambda} (z^\alpha - \Delta)^{-1} y_n(z)\mathrm{d}z - \sum_{j=-M}^M \tilde{w}_j(\tilde{z}_j^\alpha - \Delta)^{-1} y_n(\tilde{z}_j) \\
&= \mathcal{E}_{1,q}(t_n) + \widetilde{\mathcal{E}}_{2,q}(t_n).
\end{aligned} \tag{3.31}
$$

Under the induction assumption (3.29), $\|f(u_j)\|_{L^\infty}$ is bounded for $1 \le j \le m-1$, and therefore

$$\|\hat{I}_\tau f(u^{(\tau)})\|_{L^\infty(0,\,t_n;L^\infty)} \le C \sum_{j=1}^{n} \|f(u_{j-1})\|_{L^\infty} \le C, \quad 1 \le n \le m.$$

Hence, as a result of (2.15) and Lemma 3.3, we have

$$\|\mathcal{E}_{1,q}(t_n)\|_{L^\infty} + \|\widetilde{\mathcal{E}}_{2,q}(t_n)\|_{L^\infty} \le Ce^{-M/C} + Ce^{-\sqrt{2\pi d\alpha M}}. \tag{3.32}$$

This implies that

$$\|e_n^*\|_{L^\infty} \le Ce^{-M/C} + Ce^{-\sqrt{2\pi d\alpha M}} \quad \text{for } 1 \le n \le m. \tag{3.33}$$

Combining (3.33) and (3.30), and using the triangle inequality, we have

$$\begin{aligned} \|e_n\|_{L^\infty} \le & Ct_n^{\alpha-1}\tau^k + Ce^{-M/C} + Ce^{-\sqrt{2\pi d\alpha M}} \\ & + C\sum_{j=1}^{n} \tau_n (t_n - t_{j-1})^{\alpha-1} \|e_{j-1}\|_{L^\infty} \quad \text{for } 1 \le n \le m. \end{aligned} \tag{3.34}$$

By applying the discrete Gronwall's inequality in Lemma B (see Appendix B), we obtain

$$\|e_n\|_{L^\infty} \le Ct_n^{\alpha-1}\tau^k + Ce^{-M/C} + Ce^{-\sqrt{2\pi d\alpha M}} \quad \text{for } 1 \le n \le m. \tag{3.35}$$

Since $t_n \ge \tau_1 \sim \tau^k$, the above inequality furthermore implies that

$$\|e_m\|_{L^\infty} \le C\tau^{\alpha k} + Ce^{-M/C_0} + Ce^{-\sqrt{2\pi d\alpha M}}.$$

There exist positive constant τ_* and M_* (independent of m) such that when $\tau \le \tau_*$ and $M \ge M_*$, the inequality above implies

$$\|e_m\| \le 1. \tag{3.36}$$

This completes the mathematical induction on (3.29). Therefore, (3.36) holds for all $1 \le m \le N$ and, in particular, (3.35) holds for $m = N$. This proves the desired error bound (2.28) under the conditions $\tau \le \tau_*$ and $M \ge M_*$.

3.3. Proof of (2.29)**.** Under the condition $1 - \frac{1}{k} < \gamma < 1$ we have already proved that (3.36) hold for all $1 \le m \le N$, and therefore the numerical solution u_j, $j = 0, 1, \dots, N$, are bounded in $L^\infty(\Omega)$. If the stronger condition $1 - \frac{\alpha}{k} \le \gamma < 1$ holds, then $\alpha + k(\gamma - 1) \ge 0$. In this case, (3.27) implies that

$$\begin{aligned} \|\widetilde{E}_{n,1}\|_{L^\infty} \le & C\sum_{j=k}^{n} \tau_j (t_n - t_{j-1})^{\alpha-1} \sum_{i=1}^{k} \|e_{j-i}\|_{L^\infty} + C\tau^k t_n^{\alpha+k(\gamma-1)} \\ \le & C\sum_{j=k}^{n} \tau_j (t_n - t_{j-1})^{\alpha-1} \sum_{i=1}^{k} \|e_{j-i}\|_{L^\infty} + C\tau^k. \end{aligned} \tag{3.37}$$

The estimates in (3.28) (for the $k-1$ starting time levels) can be modified in the following way:

$$\begin{aligned} \|\widetilde{E}_{n,2}\|_{L^\infty} := & C\sum_{j=1}^{k-1} \int_{t_{j-1}}^{t_j} (t_n - s)^{\alpha-1} \|e_{j-1}\|_{L^\infty} \mathrm{d}s + C\sum_{j=1}^{k-1} \int_{t_{j-1}}^{t_j} (t_n - s)^{\alpha-1} \tau_j t_j^{-1} \mathrm{d}s \\ \le & C\sum_{j=1}^{k-1} \tau_j (t_n - t_{j-1})^{\alpha-1} \|e_{j-1}\|_{L^\infty} + Ct_n^{\alpha-1} \sum_{j=1}^{k-1} \tau_j \\ \le & C\sum_{j=1}^{k-1} \tau_j (t_n - t_{j-1})^{\alpha-1} \|e_{j-1}\|_{L^\infty} + C\tau_1^{\alpha} \end{aligned}$$

$$\le C\sum_{j=1}^{k-1}\tau_j(t_n-t_{j-1})^{\alpha-1}\|e_{j-1}\|_{L^\infty}+C\tau^{\frac{\alpha}{1-\gamma}}$$
$$\le C\sum_{j=1}^{k-1}\tau_j(t_n-t_{j-1})^{\alpha-1}\|e_{j-1}\|_{L^\infty}+C\tau^{k}, \tag{3.38}$$
where the last inequality requires the new condition $1-\frac{\alpha}{k}\le\gamma<1$.

The subsequent proof is the same as the proof for (2.28), except replacing $t_n^{\alpha-1}\tau^k$ by τ^k. This completes the proof of (2.29). ∎

4. Numerical tests. In this section, we present numerical results to support the theoretical analysis and illustrate the convergence of the proposed time-stepping method for nonlinear subdiffusion equations.

We consider the problem (1.1) up to time $T=1$, with a nonlinear function $f(u)=u-u^3$, which is the derivative of a double well potential $F(u)=-(1-u^2)^2/4$ and therefore generates a bounded solution satisfying $|u|\le 1$ pointwise. To investigate the performance of the numerical method for both nonsmooth and smooth initial data, we consider the following four cases:

(a) 1D and nonsmooth data: $\Omega=(0,1)$, $u_0=\chi_{[\frac12,1)}$,

(b) 1D and smooth data: $\Omega=(0,1)$, $u_0(x)=x(1-x)$,

(c) 2D and nonsmooth data: $\Omega=(0,1)^2$, $u_0=\chi_{(0,\frac12]\times(0,\frac12]}$,

(d) 2D and smooth data: $\Omega=(0,1)^2$, $u_0(x,y)=xy(1-x)(1-y)$.

The nonsmooth initial values in (a) and (c) are in $L^\infty(\Omega)$, and the smooth initial values in (b) and (d) are in $H_0^1(\Omega)\cap H^2(\Omega)$.

4.1. The convergence orders. Theorem 2.1 implies that the numerical solution given by (2.24)–(2.27) has the following error bound:

$$\|u_n-u(t_n)\|_{L^\infty}\le C\tau^k \quad \text{when } M\ge \tfrac{k^2}{2\pi d\alpha}|\ln(1/\tau)|^2.$$

We compute the errors of the numerical solutions for cases (a)-(c) by the proposed k-step method for $k=1,2,3$, respectively. The spatial discretization is done by using piecewise linear Galerkin finite element method. Unless otherwise specified, the following parameters are used in the computation:

$$\gamma=\frac34,\quad \beta=\frac{\pi}{4},\quad d=\frac{\pi}{6},\quad M=\frac{k^2c_d}{2\pi d\alpha}|\ln(1/\tau)|^2\quad\text{with}\quad c_d=\begin{cases}15 & \text{for } k=1,\\ 5 & \text{for } k=2,3,\end{cases}$$

which are needed in (2.14) and (2.17). For the stepsizes in (2.20), we simply choose $\tau_n=\big(\frac{t_{n-1}}{T}\big)^\gamma\tau$ for $n\ge 3$ in all numerical simulations.

Since the exact solution of the considered problem is not known, we compute the orders of convergence by the formula

$$\text{order of convergence}=\log\left(\frac{\|u_N^{(\tau)}-u_N^{(\tau/2)}\|_{L^\infty}}{\|u_N^{(\tau/2)}-u_N^{(\tau/4)}\|_{L^\infty}}\right)/\log(2)$$

based on the finest three meshes, where $u_N^{(\tau)}$ denotes the numerical solution at $t_N=T$ computed by using a maximal stepsize τ.

The errors of the numerical solutions to the 1D problems in (a) and (b) are presented in Tables 4.1–4.3, where we have used a sufficiently small mesh size $h=2^{-11}$ so that the error from spatial discretization is negligibly small in observing the temporal convergence rates. From Tables 4.1–4.3 we see that the proposed k-step method has kth-order convergence in time for both (a) and (b). The errors of the numerical solutions to the 2D problem in (c) are presented in Figure 4.1 (with $h=2^{-4}$), where we can see that the errors are about $O(\tau^k)$ for $k=1,2,3$, respectively.

The numerical results show that the proposed method (2.24)–(2.27) is robust for both smooth and nonsmooth initial data, consistent with the theoretical result proved in Theorem 2.1.

TABLE 4.1
Errors and convergence orders for $k = 1$ with several different $\alpha \in (0, 1)$.

α	τ	Case (a)		Case (b)	
		$\|u_N^{(\tau)} - u_N^{(\tau/2)}\|_{L^\infty}$	order	$\|u_N^{(\tau)} - u_N^{(\tau/2)}\|_{L^\infty}$	order
	1/32	2.6855e-05	–	1.0909e-05	–
	1/64	1.3288e-05	1.02	5.3944e-06	1.02
0.4	1/128	6.5086e-06	1.03	2.6409e-06	1.03
	1/256	3.1648e-06	1.04	1.2834e-06	1.04
	1/32	2.9014e-05	–	1.1821e-05	–
	1/64	1.3697e-05	1.08	5.5789e-06	1.08
0.6	1/128	6.4526e-06	1.09	2.6284e-06	1.09
	1/256	3.0491e-06	1.08	1.2425e-06	1.08
	1/32	2.2446e-05	–	9.2468e-06	–
	1/64	1.0540e-05	1.09	4.3474e-06	1.09
0.8	1/128	5.0298e-06	1.07	2.0769e-06	1.07
	1/256	2.4329e-06	1.05	1.0054e-06	1.05

TABLE 4.2
Errors and convergence orders for $k = 2$ with several different $\alpha \in (0, 1)$.

α	τ	Case (a)		Case (b)	
		$\|u_N^{(\tau)} - u_N^{(\tau/2)}\|_{L^\infty}$	order	$\|u_N^{(\tau)} - u_N^{(\tau/2)}\|_{L^\infty}$	order
	1/32	1.7254e-06	–	7.0498e-07	–
	1/64	4.2081e-07	2.04	1.7186e-07	2.04
0.4	1/128	1.0334e-07	2.03	4.2158e-08	2.03
	1/256	2.4672e-08	2.07	1.0064e-08	2.07
	1/32	2.0723e-06	–	8.5523e-07	–
	1/64	4.7937e-07	2.11	1.9796e-07	2.11
0.6	1/128	1.1154e-07	2.10	4.6103e-08	2.10
	1/256	2.6116e-08	2.09	1.0809e-08	2.09
	1/32	1.9383e-06	–	8.1334e-07	–
	1/64	4.4795e-07	2.11	1.8842e-07	2.11
0.8	1/128	1.0600e-07	2.08	4.4677e-08	2.08
	1/256	2.5515e-08	2.05	1.0769e-08	2.05

4.2. The variable stepsizes. In Figure 4.2 (left), we present the evolution of the stepsize τ_n in a time interval $[0, T]$ with a maximal stepsize $\tau = 0.1$ and different parameters $\gamma \in (0, 1)$. This illustrates how the variable stepsizes in (2.20) increase from $\tau_1 = T(\frac{\tau}{T})^{\frac{1}{1-\gamma}}$ to τ.

In Figure 4.2 (right), we present the number of total time levels N corresponding to different parameters $\gamma \in (0, 1)$ for two different maximal stepsizes, i.e., $\tau = 0.1$ and $\tau = 0.01$. From Figure 4.2 (Right) we can see that, for any fixed $\gamma \in (0, 1)$, the number of total time levels N using the stepsizes in (2.20) is equivalent to the number of total time levels using a uniform stepsize τ.

TABLE 4.3
Errors and convergence orders for $k = 3$ with several different $\alpha \in (0, 1)$.

α	τ	Case (a)		Case (b)	
		$\Vert u_N^{(\tau)} - u_N^{(\tau/2)} \Vert_{L^\infty}$	order	$\Vert u_N^{(\tau)} - u_N^{(\tau/2)} \Vert_{L^\infty}$	order
	1/8	1.1098e-05	–	4.9680e-06	–
	1/16	1.2880e-06	3.11	5.5325e-07	3.17
0.4	1/32	1.5424e-07	3.06	6.5113e-08	3.09
	1/64	1.8196e-08	3.08	7.6950e-09	3.08
	1/16	1.7711e-06	–	7.6389e-07	–
	1/32	1.9651e-07	3.17	8.4449e-08	3.18
0.6	1/64	2.2282e-08	3.14	9.5810e-09	3.14
	1/128	2.5696e-09	3.12	1.1037e-09	3.12
	1/32	2.1449e-07	–	9.3180e-08	–
	1/64	2.4151e-08	3.15	1.0531e-08	3.15
0.8	1/128	2.8142e-09	3.10	1.2323e-09	3.10
	1/256	3.3867e-10	3.05	1.4741e-10	3.06

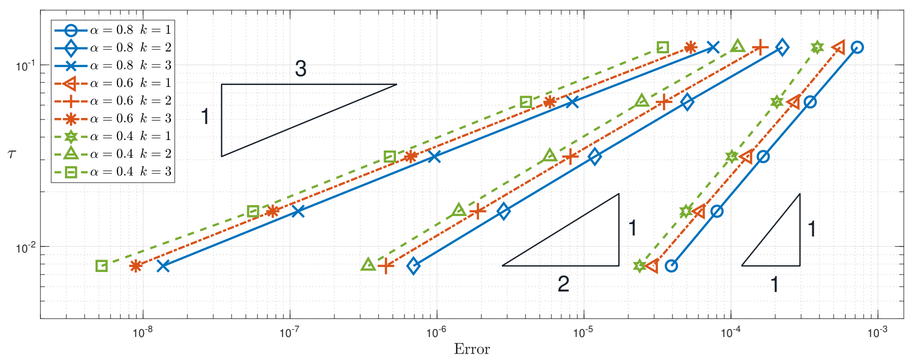

Fig. 4.1. *Errors of the numerical solutions at $T = 1$ for the 2D problem in (c).*

The errors of the numerical solutions with nonsmooth initial data in (a) are presented in Figure 4.3 for several different $\gamma \in (0, 1)$, computed with a sufficiently spatial mesh $h = 2^{-11}$. The numerical results in Figure 4.3 indicate that order reduction may happen if $\gamma < 1 - \frac{1}{k}$.

4.3. Evolution of the errors in time. In Figure 4.4 we plot the numerical solution and its errors at several different time levels for the nonlinear subdiffusion problem with nonsmooth initial data in (a) and $\alpha = 0.8$. We see that the errors of the numerical solution first increase for $t \in [0, 0.1]$ and then decrease for $t \in [0.1, 1]$.

The evolution of errors of the numerical solutions with $\alpha = 0.8$ for the four different cases in (a)–(d) are presented in Figure 4.5, where the errors are computed approximately by

$$\Vert u_n^{(\tau/\ell)} - u_n^{(\tau/16)} \Vert_{L^\infty} \quad \text{for} \quad \ell = 1, 2, 4.$$

We see that the errors of the numerical solutions with nonsmooth or smooth initial data are similar. This partly reflects the robustness of the proposed numerical method with respect to the regularity of the initial data.

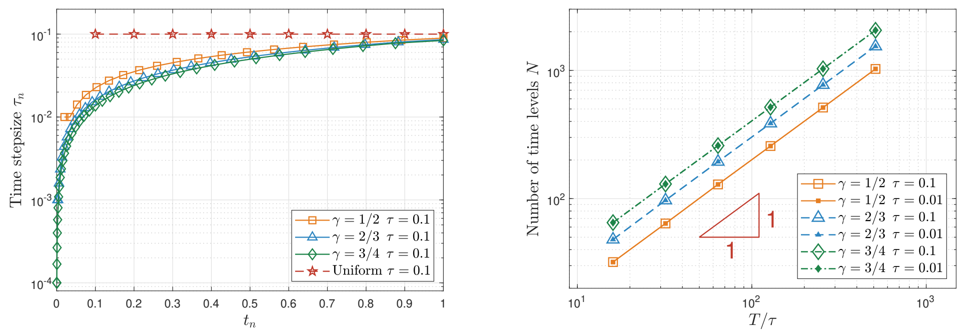

Fig. 4.2. *Left: Evolution of the variable stepsizes τ_n for several different parameters $\gamma \in (0, 1)$. Right: The number of total time levels N.*

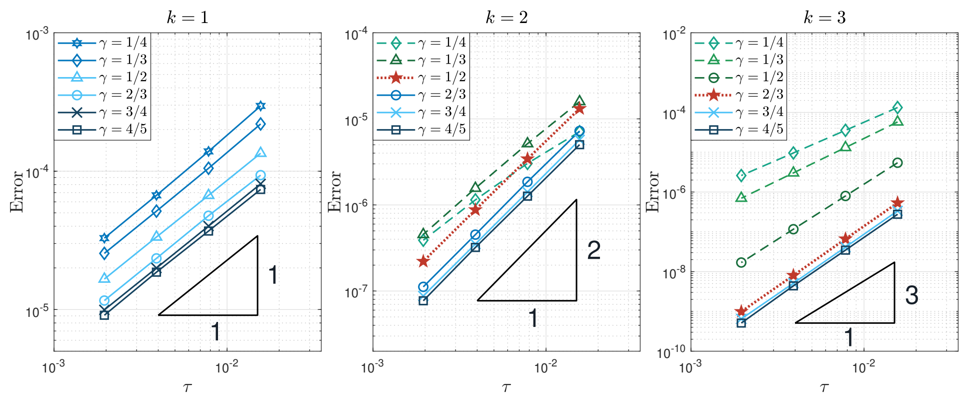

Fig. 4.3. *Errors of the numerical solutions at $T = 1$ for the nonsmooth initial data in (a), with several different parameters $\gamma \in (0, 1)$.*

5. Conclusion. We have constructed an exponential type of CQ for time discretization of the nonlinear subdiffusion equation with nonsmooth (bounded measurable) initial data, by utilizing contour integral representation of the solution, quadrature approximation of contour integrals, multistep exponential integrators for ordinary differential equations, and locally refined stepsizes to resolve the singularity at $t = 0$. Both theoretical analysis and numerical experiments show that the proposed k-step exponential CQ can have kth-order convergence in time for the solutions of the nonlinear subdiffusion equation based on natural regularity of the solution with L^∞ initial data. In this article we have focused on the analysis of semidiscretization in time. The construction and analysis of high-order spatial discretization methods for nonlinear subdiffusion equation with nonsmooth initial data are still interesting and challenging.

Appendix A: Resolvent estimates in $L^\infty(\Omega)$. It is proved in [29] that the Dirichlet Laplacian operator Δ generates a bounded analytic semigroup on $C_0(\overline{\Omega})$, satisfying the following resolvent estimate:

$$\|(z - \Delta)^{-1} v\|_{L^\infty} \leq C_\varphi |z|^{-1} \|v\|_{L^\infty} \quad \forall\, z \in \Sigma_\varphi, \ \ \forall\, v \in C_0(\overline{\Omega}), \tag{A.1}$$

where $C_0(\overline{\Omega})$ denotes the space of continuous functions on $\overline{\Omega}$ with zero boundary condition.

For any $v \in L^\infty(\Omega)$, there exists a sequence of functions $v_n \in C_0(\overline{\Omega})$ which is

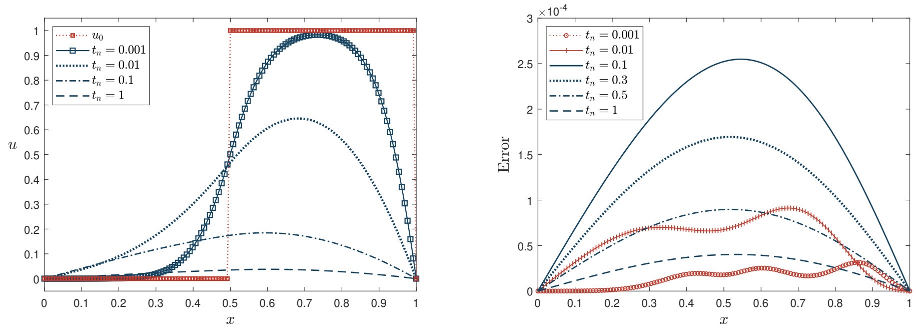

Fig. 4.4. *Numerical solutions and errors for the nonlinear subdiffusion problem with* $\alpha = 0.8$*, with nonsmooth initial data in (a), computed with* $k = 1, h = 2^{-7}$ *and* $\tau = 2^{-5}$*.*

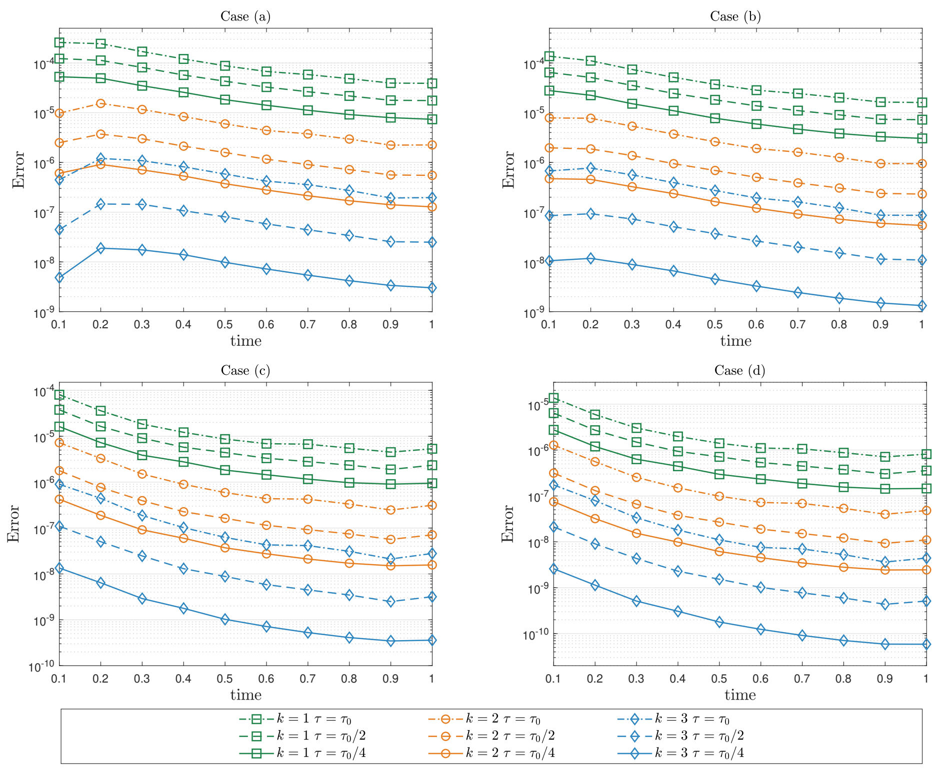

Fig. 4.5. *Evolution of errors for the four cases in (a)–(d), with* $\alpha = 0.8$ *and* $\tau_0 = 2^{-5}$*.*

bounded in $L^\infty(\Omega)$ and converges to v in $L^p(\Omega)$ for any $1 \le p < \infty$, i.e.,

$$\|v_n\|_{L^\infty} \le C\|v\|_{L^\infty} \quad \text{and} \quad \lim_{n\to\infty} \|v_n - v\|_{L^p} = 0.$$

Since $v_n \in C_0(\overline{\Omega})$, it follows from (A.1) that

$$\|(z-\Delta)^{-1}v_n\|_{L^\infty} \le C_\varphi |z|^{-1}\|v_n\|_{L^\infty} \le C_\varphi |z|^{-1}\|v\|_{L^\infty} \quad \forall\, z \in \Sigma_\varphi. \tag{A.2}$$

Since for any fixed $z \in \Sigma_\varphi$ the operator $(z-\Delta)^{-1} : L^p(\Omega) \to L^\infty(\Omega)$ is bounded when $p > \frac{d}{2}$ (see Lemma A below), and $v_n \to v$ in $L^p(\Omega)$, it follows that $(z-\Delta)^{-1}v_n$ converges to $(z-\Delta)^{-1}v$ in $L^\infty(\Omega)$. Hence, by passing to the limit $n \to \infty$ in (A.2), we obtain the desired estimate (2.5).

By using the resolvent estimate (2.5), the following estimates of the solution operators $F(t)$ and $E(t)$ can be proved (simply replacing X by $L^\infty(\Omega)$ in the proof of [11, Lemma 3.2]):

$$t^{-\alpha}\|F(t)\|_{L^\infty\to L^\infty} + t^{1-\alpha}\|F'(t)\|_{L^\infty\to L^\infty} + \|\Delta F(t)\|_{L^\infty\to L^\infty} \le C \qquad \forall\, t\in(0,T], \tag{A.3}$$

$$t^{1-\alpha}\|E(t)\|_{L^\infty\to L^\infty} + t^{2-\alpha}\|E'(t)\|_{L^\infty\to L^\infty} + t\|\Delta E(t)\|_{L^\infty\to L^\infty} \le C \quad \forall\, t\in(0,T]. \tag{A.4}$$

In the above argument we have used the following result.

Lemma A. *The operator $(z-\Delta)^{-1}: L^p(\Omega)\to L^\infty(\Omega)$ is bounded when $p>\frac{d}{2}$, and the bound is independent of $z\in\Sigma_\varphi$ for any fixed $\varphi\in(\frac{\pi}{2},\pi)$.*

Proof. Let $u=(z-\Delta)^{-1}f$. Equivalently speaking, u is the solution of the equation

$$-\Delta u = f - zu \quad \text{in } \Omega$$

under the Dirichlet boundary condition. It suffices to prove $\|u\|_{L^\infty}\le C\|f\|_{L^p}$ for $p>\frac{d}{2}$.

It is proved in [29] that the Dirichlet Laplacian operator Δ generates a bounded analytic semigroup of angle $\frac{\pi}{2}$ on $L^p(\Omega)$. The analyticity of the semigroup on $L^p(\Omega)$ implies that the operator $z(z-\Delta)^{-1}: L^p(\Omega)\to L^p(\Omega)$ is bounded, and the bound is independent of z for $z\in\Sigma_\varphi$ for any fixed $\varphi\in(\frac{\pi}{2},\pi)$; see [2, Theorem 3.7.11]. This means that

$$\|u\|_{L^p}\le C|z|^{-1}\|f\|_{L^p}.$$

The L^∞ estimate of elliptic equations (cf. [8, Theorem 8.15]) says that

$$\|u\|_{L^\infty}\le C\|f-zu\|_{L^p} \quad \text{for any fixed } p>\frac{d}{2}.$$

The two estimates above imply that

$$\|u\|_{L^\infty}\le C\|f\|_{L^p}+C|z|\|u\|_{L^p}\le C\|f\|_{L^p} \quad \text{for any fixed } p>\frac{d}{2}.$$

This proves the desired result. ∎

Appendix B: A discrete Gronwall's inequality. The following discrete Gronwall's inequality is an extension of [6, Lemma 7.1] to variable stepsizes, which plays an important role in the proof of Theorem 2.1.

Lemma B. *If $\eta_0=0$, $0\le\eta_n\le R$ for $n=1,\dots,m$, and*

$$\eta_n\le t_n^{\alpha-1}A_1+A_2+B\sum_{j=1}^n\tau_j(t_n-t_{j-1})^{\alpha-1}\eta_{j-1}, \quad n=1,\dots,m,$$

for some constants $A_1,A_2,B\ge 0$ and $\alpha>0$, then there are constants $\tau_0=\tau_0(R,B,\alpha)$ and $C=C(B,T,\alpha)$ such that the following inequality holds for $\tau\le\tau_0$:

$$\eta_n\le C(t_n^{\alpha-1}A_1+A_2), \quad n=1,\dots,m.$$

Proof. Let $\eta(t)=\eta_n$ for $t\in(t_{n-1},t_n]$. Then for $t\in(t_{n-1},t_n]$ and $n\ge 2$ there holds $t_n\sim t$, and

$$\begin{aligned}\eta(t)=\eta_n &\le t^{\alpha-1}A_1+A_2+C\sum_{j=2}^n\tau_j(t_n-t_{j-1})^{\alpha-1}\eta_{j-1}\\ &\le t^{\alpha-1}A_1+A_2+C\sum_{j=2}^n\int_{t_{j-2}}^{t_{j-1}}(t_n-s)^{\alpha-1}\eta(s)\mathrm{d}s\\ &\qquad\qquad (\text{because } t_n-t_{j-1}\sim t_n-s \text{ for } s\in(t_{j-2},t_{j-1}])\end{aligned}$$

$$
\begin{aligned}
&= t^{\alpha-1}A_1 + A_2 + C\sum_{j=1}^{n-1}\int_{t_{j-1}}^{t_j}(t_n-s)^{\alpha-1}\eta(s)\mathrm{d}s \\
&\le t^{\alpha-1}A_1 + A_2 + C\sum_{j=1}^{n-1}\int_{t_{j-1}}^{t_j}(t-s)^{\alpha-1}\eta(s)\mathrm{d}s \\
&\qquad\qquad\qquad (\text{because } (t_n-s)^{\alpha-1}\le C(t-s)^{\alpha-1} \text{ for } t\in(t_{n-1},t_n]) \\
&\le t^{\alpha-1}A_1 + A_2 + C\int_0^t(t-s)^{\alpha-1}\eta(s)\mathrm{d}s.
\end{aligned}
$$

For $t\in(0,t_1]$, the discrete Gronwall's inequality in Lemma B reduces to

$$
\eta(t)=\eta_1\le t_1^{\alpha-1}A_1+A_2\le t^{\alpha-1}A_1+A_2+C\int_0^t(t-s)^{\alpha-1}\eta(s)\mathrm{d}s.
$$

This shows that $\eta(t)$ satisfies the continuous version of Gronwall's inequality

$$
\eta(t)\le b(t)+C\int_0^t(t-s)^{\alpha-1}\eta(s)\mathrm{d}s \quad \text{for } t\in(0,t_m], \quad \text{with } b(t)=t^{\alpha-1}A_1+A_2,
$$

see [4, Lemma 1]. The continuous Gronwall's inequality implies that

$$
\eta(t)\le C(t^{\alpha-1}A_1+A_2) \quad \text{for } t\in(0,t_m].
$$

This proves the desired result in Lemma B. ∎

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