AN EXPONENTIAL SPECTRAL METHOD USING VP MEANS FOR SEMILINEAR SUBDIFFUSION EQUATIONS WITH ROUGH DATA

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Abstract. A new spectral method is constructed for the linear and semilinear subdiffusion equations with possibly discontinuous rough initial data. The new method effectively combines several computational techniques, including the contour integral representation of the solutions, the quadrature approximation of contour integrals, the exponential integrator using the de la Vallée Poussin means of the source function, and a decomposition of the time interval geometrically refined towards the singularity of the solution and the source function. Rigorous error analysis shows that the proposed method has spectral convergence for the linear and semilinear subdiffusion equations with bounded measurable initial data and possibly singular source functions under the natural regularity of the solutions.

Key words. Semilinear subdiffusion equation, singularity, spectral method, exponential integrator, VP means, geometric decomposition, contour integral, quadrature approximation, convolution quadrature

AMS subject classifications. 65M12, 35K55

1. Introduction. We consider the semilinear subdiffusion equation in a bounded Lipschitz domain $\Omega \subset \mathbb{R}^d$ up to a given time $T > 0$, under the Dirichlet boundary condition, i.e.,

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

where $f : \mathbb{R} \times \mathbb{R}^d \times \mathbb{R}_+ \to \mathbb{R}$ and u_0 are the given nonlinear function and initial value, and $\partial_t^\alpha u$ denotes the Caputo fractional derivative of order $\alpha \in (0,1)$. The subdiffusion equations which can model the sublinear growth of mean squared particle displacement have generated much interests from physicists, engineers and applied mathematicians in developing new computational methods and rigorous numerical analyses because of their excellent capability in modelling the anomalous transport processes. The construction and analysis of high-order computational methods for the subdiffusion equations, especially for the semilinear subdiffusion equation, have been challenging due to the possible singularity of the solution and the source function at $t = 0$.

In general, for the linear subdiffusion equation with initial value $u_0 \in H_0^1(\Omega) \cap H^2(\Omega)$ and a temporally smooth source function $f(x,t)$ (independent of u), the solution generally exhibits the following type of weak singularity at $t = 0$ (see [15, Theorem 1]):

$$\|\partial_t^m (u(\cdot,t) - u_0)\|_{L^2} \le C_m t^{\alpha - m} \quad \text{for } m \ge 0. \tag{1.2}$$

Under this limited regularity condition, the classical L1, L2, dG and convolution quadrature (CQ) with a uniform stepsize generally have first-order convergence; for example, see [12, 13, 33, 40]. The analyses in [17, 19, 35, 37] show that the L1 and L2

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methods, and a low-order dG time-stepping method, can have the desired optimal-order convergence by using graded stepsizes locally refined towards $t = 0$. The extension of these low-order convergence results to the semilinear subdiffusion equation may be established by using the fractional version of discrete Gronwall's inequalities in [14, 24, 25]. The sharp pointwise-in-time error bounds on quasi-graded temporal meshes with arbitrary degree of grading are obtained in [16] using method of upper and lower solutions for L1 scheme. Higher-order sub-optimal convergence in time was proved for the dG time-stepping method in [34] under condition (1.2) and some additional regularity assumptions such as $\partial_t u \in L^2(0,T;H^2(\Omega))$, which generally requires the initial value to satisfy $u_0 \in H^{5/2}(\Omega) \cap H_0^1(\Omega)$ plus a compatibility condition $\Delta u_0 = 0$ on $\partial\Omega$. In the case $u_0 = 0$, high-order convergence of the Runge–Kutta convolution quadrature was proved in [2].

The extension of the above-mentioned results to rough initial data in $L^p(\Omega)$ with $1 \le p \le \infty$ (without any differentiability), using graded stepsizes to improve the convergence orders, is still challenging due to the stronger singularity in this case (see [15, Theorem 1]), i.e.,

$$\|\partial_t^m u(\cdot,t)\|_{L^p} \le C_m t^{-m} \quad \text{for } m \ge 0. \tag{1.3}$$

Under this regularity condition, the L1, L2 and CQ schemes with a uniform stepsize and appropriate initial corrections can have high-order convergence at time levels far away from $t = 0$, i.e.,

$$\|u(\cdot,t_n) - u_n\|_{L^p} \le C t_n^{-k} \tau^k, \tag{1.4}$$

where u_n denotes the numerical solution using a uniform stepsize τ. The results were established in [13,31,40] in the L^2-norm framework, i.e., with error estimates in the L^2 norm and initial data in $L^2(\Omega)$, by comparing the numerical solution with the solution through their Laplace transform representations, a framework developed by Lubich for the analysis of CQ for convolution integrals; see [27–29]. Nevertheless, the analyses can be naturally extended to the L^p-norm framework by using the corresponding resolvent estimate in $L^p(\Omega)$, i.e.,

$$\|(z-\Delta)^{-1}\|_{L^p(\Omega)\to L^p(\Omega)} \le C|z|^{-1}, \quad 1 \le p \le \infty,$$

which holds for both the Laplacian Δ and the finite element discrete Laplacian Δ_h; see [20, 21]. However, these high-order convergence results only hold for the linear subdiffusion equation with a given temporally smooth source function.

The extension of the high-order methods to the semilinear subdiffusion equation with nonsmooth initial data is still challenging. The main difficulty in the numerical solution of the semilinear subdiffusion equation is that the source function $f(u(x,t),x,t)$ also becomes singular at $t = 0$ due to the singularity of $u(x,t)$. In this case, the regularity of the solution and the source function is

$$\|\partial_t^m (u(\cdot,t) - u_0)\|_{L^\infty} + \|\partial_t^m f(u(\cdot,t),\cdot,t)\|_{L^\infty} \le C_m t^{\alpha-m} \quad \text{for } m \ge 0 \tag{1.5}$$

and

$$\|\partial_t^m u(\cdot,t)\|_{L^\infty} + \|\partial_t^m f(u(\cdot,t),\cdot,t)\|_{L^\infty} \le C_m t^{-m} \quad \text{for } m \ge 0 \tag{1.6}$$

for initial data in $H_0^1(\Omega) \cap C^2(\overline{\Omega})$ and $L^\infty(\Omega)$, respectively; see [22, 39]. The convergence of the backward Euler CQ was not affected by the singularity of the source function, as shown in [14] and [1] for initial data in $H_0^1(\Omega) \cap H^2(\Omega)$ and $H^s(\Omega)$, $s > 0$, respectively. However, the convergence of higher-order CQs can be affected by the singularity of the source function at $t = 0$. In particular, the analysis and numerical experiments in [39] show that the convergence order of high-order BDF-CQs, using a uniform stepsize with appropriate initial corrections, is at most $1 + 2\alpha$ for general initial data in $H_0^1(\Omega) \cap C^2(\overline{\Omega})$. More recently, a k-step exponential CQ was proposed in [22] to achieve kth-order convergence for semilinear subdiffusion equation with initial data in $L^\infty(\Omega)$, where k is an arbitrary prescribed positive integer which determines the numerical scheme and the convergence order.

The above-mentioned methods all have fixed convergence orders. The development of spectral methods, which converge faster than $O(N^{-k})$ for any fixed positive integer k (where N denotes the degrees of freedom in the time discretization), is still challenging for the subdiffusion equation with singular solutions and source functions. Many efficient spectral methods for the fractional ordinary and partial differential equations have been proposed and analyzed:

- A new multi-domain spectral method for high-order time discretizations of fractional ordinary differential equations (ODEs) and the subdiffusion equation was proposed in [4]. The stability of the method was studied by identifying the method as a generalized linear method. The rigorous analysis of its spectral convergence for the subdiffusion equation with rough initial data still remains challenging.
- A class of spectral collocation methods based on the generalized Jacobi functions was proposed in [42, 43] for some fractional differential equations. The approximation errors of the generalized Jacobi polynomials in weighted Sobolev spaces, as well as the convergence of the spectral Petrov–Galerkin method for fractional ordinary differential equations (ODEs), were presented in [7]. The current analysis requires some fractional derivatives of the solution to be smooth, which is true for some fractional ODEs but cannot be readily extended to the subdiffusion equation. The rigorous analysis of this class of methods for the subdiffusion equation with rough initial data still remains challenging.
- The generalied Jacobi polynomials were also used for calculating the eigenvalues of the space-fractional differential equations in [5] and for determining the superconvergence points of fractional spectral interpolations in [44].
- A class of Müntz spectral Galerkin methods were proposed and analyzed in [10, 11] based on the Müntz polynomials and weighted Sobolev spaces. The methods have spectral convergence for solutions with the following regularity:
  $$t^{-1+m}\partial_t^m[u(x,t^{1/\lambda})] \in L^2(0,T;H_0^1(\Omega)) \quad \forall\, m \geq 0. \tag{1.7}$$
  This covers a wide class of solutions, including solutions in the form of
  $$u(x,t) = \sum_{j=1}^{\infty} t^{j\alpha}\phi_j(x),$$
  which can be approximated with spectral convergence by choosing $\lambda = 1/\alpha$. For more general solutions of the subdiffusion equation with initial data in $H_0^1(\Omega) \cap H^2(\Omega)$, when the solutions have the regularity in (1.2) but may not satisfy condition (1.7), the Müntz spectral Galerkin methods can still have a fixed high order of convergence by choosing a sufficiently small parameter λ.
- A class of log-orthogonal spectral methods for the subdiffusion equation was proposed and analyzed in [8] by using the log-orthogonal polynomials introduced in [6]. It is shown that the method can have spectral convergence if the initial value satisfies $u_0 \in \dot{H}^3(\Omega)$, which is equivalent to requiring

$u_0 \in H_0^1(\Omega) \cap H^3(\Omega)$ plus one compatibility condition $\Delta u_0 = 0$ on $\partial\Omega$.

As far as we know, the following questions are still unsolved in the development of spectral methods for the subdiffusion equations.

- The current error analysis of spectral methods for the subdiffusion equation requires the initial data to be smoother than $H_0^1(\Omega) \cap H^2(\Omega)$ and satisfying some compatibility conditions, or satisfying a regularity condition in the form of (1.5). The construction of spectral methods for the semilinear subdiffusion equation with rough initial data in $L^\infty(\Omega)$ with strong singularity in the form of (1.6) is still challenging.
- The existing error estimates for the spectral methods are all for the linear subdiffusion equation based on the Hilbert space framework. The extension of the error analysis for the spectral methods to the semilinear subdiffusion equation, with nonlinear source functions which may not be globally Lipschitz continuous, requires error estimates in the L^∞-norm based Banach space framework and therefore still remains open. There are few analysis of spectral methods in the L^∞-norm framework. We are only aware of the L^∞-norm analysis of spectral methods in [23] by the effective maximum principle of spatial discretizations. The techniques cannot be applied to the time discretization of the subdiffusion equation in the presence of singularity.

These questions are addressed in this article.

We propose a new spectral method for the semilinear subdiffusion equation with rough initial data in $L^\infty(\Omega)$ under the natural regularity condition (1.6), based on quadrature approximations to the contour integral representation of the solution, the exponential integrator using the de la Vallée Poussin means (i.e., VP means, see [38]), and error estimates via a fixed-point argument in an L^∞-norm framework. The contour integral approximation techniques were used in [26] and [9] for evaluating exponential-type of operators and for solving linear convection–diffusion equations, respectively. The techniques were also used in the construction of a high-order backward extrapolated multi-step exponential convolution quadrature for the semilinear subdiffusion equation in [22]. However, the method in [22] only has a fixed order of convergence and cannot be extended to a spectral method directly due to the following three challenges: (1) The temporal Lagrange interpolation used in [22] is not stable in the L^∞ norm as the degrees of freedom tend to infinity; (2) The integrals of the exponential function times the Lagrange basis is difficult to be evaluated analytically when the degree of the polynomial is large; (3) The source function is singular at $t = 0$ and therefore the Lagrange interpolation on the whole time interval does not have uniform high-order convergence.

We overcome these difficulties by utilizing an exponential type of spectral method in terms of the interpolation polynomial VP means on subintervals that are geometrically refined towards $t = 0$ according to the singularity of the solution and the source function. We derive analytical formulas for the exponential integrals arising from the proposed method by utilizing the differentiation properties of the Jacobi polynomials, and prove the spectral convergence of the proposed method based on the natural regularity condition in (1.6) using the L^∞ stability of the polynomial VP means and their approximation properties on the geometrically refined subintervals. The spectral convergence in the L^∞ norm is established, which allows us to handle nonlinear source functions which are only locally Lipschitz continuous (rather than globally Lipschitz continuous). These results make the proposed method practically computable and spectrally convergent for rough solutions of the semilinear subdiffusion equation in the most general setting.

In view of the equivalence between CQs and their Laplace transform representations, e.g., the Runge–Kutta (or BDF) CQ for a parabolic or subdiffusion equation is equivalent to applying the Runge–Kutta method (or BDF) method to the ODE arising from the Laplace transform representation of the solution (as shown in [30]), the exponential spectral method proposed in this article can also be viewed as a contour integral approximation to a spectrally convergent CQ constructed by utilizing an exponential integrator for the ODE arising from the Laplace transform representation of the solution, and by utilizing VP means of the source function on geometrically refined subintervals adapted to the singularity at $t = 0$.

The rest of this article is organized as follows. The quadrature approximation of the mild solution and the uniform polynomial approximation of functions by VP means are presented in Section 2. The new spectral method and its error analysis for the linear subdiffusion equation with a possibly singular source function are presented in Section 3. The new spectral method and its error analysis for the semilinear subdiffusion equation are presented in Section 4. Numerical experiments are presented in Section 5 to illustrate the spectral convergence of the proposed method for linear and semilinear subdiffusion problems with rough initial data in $L^\infty(\Omega)$. Concluding remarks are presented in Section 6.

2. Construction of the spectral method. In this section, we introduce the several ingredients we use to construct the spectral method, including the contour integral representation of the solution, quadrature approximation to the contour integrals, polynomial approximation by the VP means, and the exponential integrator using VP means. The construction of the spectral method is discussed at the end of this section, while the complete algorithms are presented in the next two sections for the linear and semilinear subdiffusion equations, respectively.

2.1. Bounded mild solutions to the subdiffusion equation. For the simplicity of notations, we denote $u(t) = u(\cdot, t)$ for any function u defined on $\Omega \times (0, T]$. A function $u \in L^\infty(0, T; L^\infty(\Omega)) \cap C([0, T]; L^2(\Omega))$ is called a bounded mild solution of (1.1) if it satisfies the following equation

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

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

$$F(t) = \frac{1}{2\pi i} \int_{\mathrm{Re}(z)=\sigma} z^{\alpha-1}(z^\alpha - \Delta)^{-1} e^{zt}\, \mathrm{d}z$$
$$E(t) = \frac{1}{2\pi i} \int_{\mathrm{Re}(z)=\sigma} (z^\alpha - \Delta)^{-1} e^{zt}\, \mathrm{d}z,$$

with an arbitrary parameter $\sigma > 0$. The paths of integration in the expressions of $F(t)$ and $E(t)$ can be respectively deformed to the following two contours on the complex plane:

$$\Gamma_\lambda = \{\lambda(1 - \sin(\beta + is)) : s \in \mathbb{R}\} \quad \text{and} \quad \Gamma_{\tilde{\lambda}} = \{\tilde{\lambda}(1 - \sin(\beta + is)) : s \in \mathbb{R}\}, \tag{2.2}$$

where $\beta \in (0, \varphi - \frac{\pi}{2})$, $\varphi \in (\frac{\pi}{2}, \pi)$ and $\lambda, \tilde{\lambda} > 0$ can be arbitrary fixed parameters. These contours are contained in the region between the two sectors $\Sigma_\varphi = \{z \in \mathbb{C} :$

$|\arg(z)| \le \varphi\}$ and $\lambda + \Sigma_{\beta+\frac{\pi}{2}}$; see [22, Figure 2.1]. Therefore,

$$\mathrm{Re}(z) \sim -|z| \quad \text{and} \quad |\mathrm{Im}(z)| \sim |\mathrm{Re}(z)| \quad \text{for} \ z \in \Gamma_\lambda \cup \Gamma_{\tilde{\lambda}}.$$

The representation of the solutions to the subdiffusion equation in (2.1) has been used in analyzing the regularity of solutions and the error of numerical approximations in [14, 22, 31, 39, 40]. The integration contours in the form of (2.2) have been used in approximating exponential-type functions of elliptic operators in [9, 26].

It is known that the resolvent operators $(z^\alpha - \Delta)^{-1}$ of the Dirichlet Laplacian satisfy the following estimate for some constant $C > 0$ (for example, see [22, Appendix A]):

$$\|(z^\alpha - \Delta)^{-1}\|_{L^\infty \to L^\infty} \le C(1 + |z|)^{-\alpha} \ \text{for} \ z \in \Gamma_\lambda. \tag{2.3}$$

As a result of the resolvent estimate in (2.3), the solution operators $F(t)$ and $E(t)$ were proved to satisfy the following estimates (cf. [22, Lemma 3.1]):

$$\|F(t)\|_{L^\infty \to L^\infty} \le C \quad \text{and} \quad \|E(t)\|_{L^\infty \to L^\infty} \le Ct^{\alpha-1}. \tag{2.4}$$

By using these properties of the solution operators, it can be shown that equation (1.1) indeed has a bounded mild solution if the one of the following two conditions is satisfied:

(1) The nonlinear function $f(u)$ is Lipschitz continuous with respect to u. In this case, the proof of well-posedness in [14] is still valid if the underlying space $L^2(\Omega)$ is replaced by $L^\infty(\Omega)$, as the proof only requires using the resolvent estimate in (2.3).
(2) The nonlinear function $f(u) = -F'(u)$ is the derivative of a double-well potential $F(u)$ with two wells at $\pm\alpha$, and the initial value satisfies that $|u_0| \le \alpha$. For example, $f(u) = (u - u^3)/\varepsilon^2 = -F'(u)$ with $F(u) = (1 - u^2)^2/(4\varepsilon^2)$ being the Ginzburg–Landau potential. In this case, the maximum principle of the subdiffusion equation (cf. [41, Theorems 3.1–3.2], [32, Theorem 2.1] and [18]) guarantees the boundedness of the solution, i.e., $|u(x, t)| \le \alpha$.

In view of these results, we simply assume that the semilinear subdiffusion equation has a bounded mild solution and propose a class of spectral methods for the linear and semilinear problems, respectively, with rigorous analysis for the existence, uniqueness and spectral convergence of the numerical approximations.

Throughout this article, we denote by C a generic positive constant that may be different at different occurrences but is independent of the number N_m, $N_1(m)$ of subintervals, the time level t_n, and the number M of quadrature points for approximating the contour integrals.

2.2. Quadrature approximation of the mild solution. By substituting the contour integral expressions of $F(t)$ and $E(t)$ into (2.1), and make a change of variable in the first integral of (2.1), we can express the mild solution as

$$\begin{aligned} u(t) = &\frac{1}{2\pi i} \int_{\Gamma_\lambda} e^z z^{\alpha-1} (z^\alpha - t^\alpha \Delta)^{-1} u_0 \, \mathrm{d}z \\ &+ \frac{1}{2\pi i} \int_{\Gamma_{\tilde{\lambda}}} (z^\alpha - \Delta)^{-1} \int_0^t e^{z(t-s)} f(u(s), \cdot, s) \, \mathrm{d}s \, \mathrm{d}z, \end{aligned} \tag{2.5}$$

It is also known that the two contour integrals on the right-hand side of (2.5) can be approximated by a quadrature which has spectral convergence with respect to the number of quadrature points, i.e.,

$$
\begin{aligned}
u(t) = &\sum_{j=-M}^{M} \omega_j e^{z_j} z_j^{\alpha-1}(z_j^\alpha - t^\alpha \Delta)^{-1} u_0 + \mathcal{E}_{1,q}(t) \\
&+ \sum_{j=-M}^{M} \tilde{\omega}_j (\tilde{z}_j^\alpha - \Delta)^{-1} y(\tilde{z}_j, t) + \mathcal{E}_{2,q}(t),
\end{aligned} \tag{2.6}
$$

where $2M+1$ quadrature points are used, (ω_j, z_j) and $(\tilde{\omega}_j, \tilde{z}_j)$ are two pairs of quadrature weights and nodes, with $\mathcal{E}_{1,q}(t)$ and $\mathcal{E}_{2,q}(t)$ denoting the remainders of the quadrature approximations, and $y(z,t) = \int_0^t e^{z(t-s)} f(u(s), \cdot, s)\,\mathrm{d}s$ is the solution of the following ordinary differential equation (ODE):

$$
\frac{\mathrm{d}}{\mathrm{d}t} y(z,t) = z y(z,t) + f(u(t), \cdot, t). \tag{2.7}
$$

The explicit expressions of the quadrature weights and nodes can be found in [22]. Moreover, the remainders satisfy the estimates in the following lemma.

Lemma 2.1 (cf. [22, Lemma 3.3]). *If* $\|f(u,\cdot,\cdot)\|_{L^\infty(0,t;L^\infty(\Omega))} \le C$ *then*

$$
\|\mathcal{E}_{1,q}(t)\|_{L^\infty(\Omega)} + \|\mathcal{E}_{2,q}(t)\|_{L^\infty(\Omega)} \le C e^{-\sqrt{M}/C}. \tag{2.8}
$$

The representation of the mild solution by the discrete contour integrals in (2.6)–(2.7) was proposed in [22] for solving the semilinear subdiffusion equation by an exponential CQ with k-step extrapolation, which can only have kth-order convergence with a fixed $k \ge 1$. In the next subsection, we propose a spectrally convergent method based on the expression in (2.6)–(2.7) and a uniform polynomial interpolation technique using the VP means.

2.3. Uniform polynomial approximation by VP means. We denote the space of polynomials of degree $\le m$ on the interval $[-1,1]$ by $P_m([-1,1])$, and define the L^∞-norm polynomial approximation error as

$$
E_m(g)(x) := \inf_{p \in P_m} \|g(x,\cdot) - p(\cdot)\|_{L^\infty(-1,1)} \quad \text{for } g \in C(\overline{\Omega} \times [-1,1]). \tag{2.9}
$$

In the approximation theory, the following results are known (see [3, (5.4.16)]).

Lemma 2.2. *For* $0 \le k \le m$ *and* $g \in C^k([-1,1]; L^\infty(\Omega))$ *the following estimates hold:*

$$
\begin{aligned}
|E_m(g)(x)| &\le C_k m^{-k} \|g(x,\cdot)\|_{C^k([-1,1])}, \\
\|E_m(g)\|_{L^\infty(\Omega)} &\le C_k m^{-k} \|\partial_t^k g\|_{C([-1,1];L^\infty(\Omega))}.
\end{aligned} \tag{2.10}
$$

It is known that the Lagrange interpolation operator $I_m : C([-1,1]) \to P_m([-1,1])$ is not stable with respect to m, i.e.,

$$
\|I_m g\|_{C([-1,1])} \le C \log(m) \|g\|_{C([-1,1])}, \tag{2.11}
$$

where the logarithmic factor in m cannot be removed. This significantly affects the stability of the spectral methods based on the Lagrange interpolation for nonlinear problem, for which the error estimates require using Gronwall's inequality. We shall use a different interpolation technique in our spectral method, called the polynomial VP means, which turns out to be not only stable in $C([-1,1]; L^\infty(\Omega))$ but also convenient for the practical computations in combination with exponential integrators.

Let $t_{m,1} < t_{m,2} < \cdots < t_{m,m}$ be the m zeros of the normalized Jacobi polynomial $J_m^{\alpha,\beta}(t)$ of degree m on the interval $[-1,1]$, with the Jacobi weight $\omega^{\alpha,\beta} = (1-t)^\alpha(1+$

$t)^\beta$. The following polynomial VP means of a function $g \in C([-1,1])$ will be used:

$$V_m^r g(t) = \sum_{i=1}^{m} g(t_{m,i})\Phi_{m,i}^r(t) \quad \text{for } g \in C([-1,1]), \tag{2.12}$$

where

$$\Phi_{m,i}^r(t) = \frac{\sum_{j=0}^{m+r-1} \mu_{m,j}^r J_j^{\alpha,\beta}(t_{m,i}) J_j^{\alpha,\beta}(t)}{\sum_{j=0}^{m-1} [J_j^{\alpha,\beta}(t_{m,i})]^2}, \quad j = 1, \dots m, \tag{2.13}$$

with

$$\mu_{m,j}^r := \begin{cases} 1 & \text{if} \quad 0 \le j \le m-r, \\ \frac{m+r-j}{2r} & \text{if} \quad m-r < j < m+r, \\ 0 & \text{if} \quad j \ge m+r. \end{cases} \tag{2.14}$$

For $|\alpha| = |\beta| = \frac{1}{2}$, the VP means enjoy the interpolation properties, i.e., $V_m^r g(t_{m,i}) = g(t_{m,i})$ for $i = 1, \dots, m$.

In this article, we simply choose $r \le \theta m$ for some fixed $\theta \in (0,1)$. Then the approximation errors of the polynomial VP means are given in the following lemma, which shows that the L^∞-stability constant of the polynomial VP means is independent of the polynomial degree.

Lemma 2.3 ([38, Theorem 3.2]). *For sufficiently large positive integers m and r satisfying $r \le \theta m$, the following estimates hold:*

$$\|V_m^r g\|_{C([-1,1];L^\infty(\Omega))} \le C \sup_{1 \le i \le m} \|g(t_{m,i})\|_{L^\infty(\Omega)} \quad \textit{for } g \in C([-1,1]; L^\infty(\Omega)), \tag{2.15}$$

$$\|g - V_m^r g\|_{C([-1,1];L^\infty(\Omega))} \le C \|E_{m-r}(g)\|_{L^\infty(\Omega)} \quad \textit{for } g \in C([-1,1]; L^\infty(\Omega)), \tag{2.16}$$

for some constant C which does not depend on m.

2.4. The exponential integrator using VP means. The only unknown on the right-hand side of (2.6) is $y(\tilde{z}_j, t)$, which we shall approximate by the exponential integrator

$$y(\tilde{z}_j, t_{ni}) = e^{\tilde{z}_j (t_{ni} - t_{n-1})} y(\tilde{z}_j, t_{n-1}) + \int_{t_{n-1}}^{t_{ni}} e^{\tilde{z}_j (t_{ni} - s)} V_m^r f(u(s), \cdot, s)\, \mathrm{d}s \tag{2.17}$$

at the finitely many internal nodes $t_{ni} \in (t_{n-1}, t_n]$, $i = 1, \dots, m$, where the polynomial VP mean $V_m^r f(u(s), \cdot, s)$ only depends on the finitely many values $f(u(t_{ni}), \cdot, t_{ni})$, $i = 1, \dots, m$.

Since the VP means can be expressed as linear combinations of the Jacobi polynomials, the integral in (2.17) can be evaluated analytically by using the following formula:

$$\int_{-1}^{t} e^{z(t-s)} J_m^{\alpha,\beta}(s)\, \mathrm{d}s = \sum_{k=0}^{m} \frac{d_{m,k}^{\alpha,\beta}}{z^{k+1}} \sqrt{\frac{\gamma_{m-k}^{\alpha+k,\beta+k}}{\gamma_m^{\alpha,\beta}}} (-J_{m-k}^{\alpha+k,\beta+k}(t) + e^{z(t+1)} J_{m-k}^{\alpha+k,\beta+k}(-1)). \tag{2.18}$$

This formula can be derived by using integration by parts and the following differentiation property of the Jacobi polynomials ([36, (3.101)]):

$$\partial_t^k J_m^{\alpha,\beta}(t) = d_{m,k}^{\alpha,\beta} \sqrt{\frac{\gamma_{m-k}^{\alpha+k,\beta+k}}{\gamma_m^{\alpha,\beta}}} J_{m-k}^{\alpha+k,\beta+k}(t),$$

where

$$d_{m,k}^{\alpha,\beta} = \frac{\Gamma(m+k+\alpha+\beta+1)}{2^k\Gamma(m+\alpha+\beta+1)},$$

$$\gamma_m^{\alpha,\beta} = \frac{2^{\alpha+\beta+1}\Gamma(m+\alpha+1)\Gamma(m+\beta+1)}{(2m+\alpha+\beta+1)m!\Gamma(m+\alpha+\beta+1)}.$$

By a simple scaling transformation, we can use formula (2.18) to compute the integral in (2.17) in terms of the values $f(u(t_{ni}),\cdot,t_{ni})$, $i=1,\dots,m$. Then, by substituting the computed values $y(\tilde{z}_j,t_{ni})$ into (2.6), we can obtain the desired spectral method. The complete algorithms are presented in the next two sections for the linear and semilinear subdiffusion equations, respectively.

3. The linear problem with a singular source. In this section, we present the spectral algorithm for the linear subdiffusion equation with a given source function $f(x,t)$ which may be singular at $t=0$ (but is independent of u).

Since the solution representation in (2.6)–(2.7) does not depend on the history values of the solution, i.e., it only depends on the value of $y(z,t)$ which satisfies the ODE problem in (2.7), which does not contain history integrals, the case $T>1$ can be reduced to the case $T=1$ by dividing the time interval $[0,T]$ into several parts. The case $T<1$ can be converted to the case $T=1$ via a temporal scaling transformation. Therefore, without loss of generality, we focus on the case $T=1$ and consider the subdiffusion equation on the unit time interval $[0,1]$.

If the source function is smooth, i.e., $f\in C^\infty([0,1];L^\infty(\Omega))$, then we can approximate the source function f by its VP mean $V_m^r f$ on the whole interval $[0,1]$. In particular, let $t_{m,1}<t_{m,2}<\cdots<t_{m,m}$ be the zeros of the Jacobi polynomial $J_m^{\alpha,\beta}(t)$ of degree m on the time interval $[0,1]$. For any fixed $t\in[0,1]$ we can approximate $y(z,t)$ by

$$y_m(z,t) = \int_0^t e^{z(t-s)} V_m^r f(s)\,\mathrm{d}s, \tag{3.1}$$

which can be evaluated exactly by using formula (2.18). By substituting (3.1) into (2.6) and dropping the two remainders $\mathcal{E}_{1,q}(t)$ and $\mathcal{E}_{2,q}(t)$, we obtain the following algorithm for any $t\in[0,1]$:

$$u_m(t) = \sum_{j=-M}^{M} \omega_j e^{z_j} z_j^{\alpha-1}(z_j^\alpha - t^\alpha\Delta)^{-1}u_0 + \sum_{j=-M}^{M}\tilde{\omega}_j(\tilde{z}_j^\alpha-\Delta)^{-1}y_m(\tilde{z}_j,t). \tag{3.2}$$

The error bound of this method is an immediate consequence of Lemma 2.1, Lemma 2.2 and Lemma 2.3 (with $r\le\theta m$ for some fixed parameter $0<\theta<1$). We present the result in the following theorem and omit the proof.

Theorem 3.1. *Let $u_0\in L^\infty(\Omega)$ and $f\in C^\infty([0,1];L^\infty(\Omega))$. Then the numerical solution defined in* (3.1)–(3.2) *has the following error bound for the linear subdiffusion equation:*

$$\max_{t\in[0,1]}\|u(t)-u_m(t)\|_{L^\infty(\Omega)} \le C_k m^{-k} + Ce^{-\sqrt{M}/C}, \tag{3.3}$$

which holds for all fixed integer $k\ge1$, all M and all sufficiently large m.

We are more interested in the development of high-order methods for the subdiffusion equation with a source function singular at $t=0$. This is often the case when the source function is related to the solution of a subdiffusion equation. The strength of such a singularity at $t = 0$ can be characterized by the following condition with a parameter $\gamma \in (0, 1]$:

$$\|(t^\gamma \partial_t)^k f(\cdot, t)\|_{L^\infty(\Omega)} \le C_k \text{ for } k \ge 0 \text{ and } t \in (0, 1]. \tag{3.4}$$

The larger value of γ, the stronger of the singularity.

For a source function which exhibits a singularity at $t = 0$ in the form of (3.4), we choose a fixed parameter $\lambda > 1$ and divide the time interval $[0, 1]$ into N subintervals, i.e.,

$$I_1 = [t_0, t_1] := [0, \lambda^{1-N}] \quad \text{and} \quad I_n = (t_{n-1}, t_n] := (\lambda^{n-1-N}, \lambda^{n-N}], \quad 2 \le n \le N,$$

where $N = N_m$ can be any integer satisfying $\lim_{m\to\infty} N_m/\log m = \infty$ (this requirement will become clear in the error analysis). On each subinterval I_n, we approximate the source function $f(\cdot, t)$ by its VP means $V_m^r f(\cdot, t)$ and substitute the value

$$y_n(z) = e^{z(t_n - t_{n-1})} y_{n-1}(z) + \int_{t_{n-1}}^{t_n} e^{z(t_n - s)} V_m^r f(s)\, \mathrm{d}s \tag{3.5}$$

into (2.6). Then, by dropping the two remainders $\mathcal{E}_{1,q}(t)$ and $\mathcal{E}_{2,q}(t)$ in (2.6), we obtain the following algorithm:

$$u_n = \sum_{j=-M}^{M} \omega_j e^{z_j} z_j^{\alpha-1} (z_j^\alpha - t_n^\alpha \Delta)^{-1} u_0 + \sum_{j=-M}^{M} \tilde{\omega}_j (\tilde{z}_j^\alpha - \Delta)^{-1} y_n(\tilde{z}_j). \tag{3.6}$$

The algorithm in (3.5)–(3.6) only requires polynomial interpolation based on the VP means, the evaluation of the exponential integrals in (3.5), and the solution of the linear systems associated to the operators $z_j^\alpha - \Delta$ and $\tilde{z}_j^\alpha - \Delta$. This is different from the spectral method for the semilinear problem to be presented in the next section, which requires solving certain nonlinear systems by fixed-point iterations or the Newton iterations.

For the linear problem with singular source function, the accuracy of the numerical approximation by (3.6) is guaranteed by the following theorem.

Theorem 3.2. *Let $u_0 \in L^\infty(\Omega)$ and assume that the source function $f(x, t)$ satisfies the regularity condition in* (3.4)*. Let u_n, $n = 1, \dots, N$ be the numerical solutions given by* (3.5)–(3.6) *with $N = N_m$ satisfying*

$$\lim_{m\to\infty} \frac{N_m}{\log(m)} = \infty. \tag{3.7}$$

Then the following error bound holds (for all integer $k \ge 1$, all M and all sufficiently large m.):

$$\max_{1\le n\le N} \|u(t_n) - u_n\|_{L^\infty(\Omega)} \le C_k m^{-k} + C e^{-\sqrt{M}/C}. \tag{3.8}$$

Remark 3.1. The total number of degrees of freedom in the time discretization is mN with $N = N_m$ satisfying condition (3.7). By choosing a moderate growing N_m, such as $N_m = m/2$, the total number of degrees of freedom is $O(m^2)$ while the error of the numerical approximation is $O(m^{-k})$ for arbitrarily large k. This means that the proposed method has spectral convergence (i.e., arbitrarily large convergence orders) with respect to the total number of degrees of freedom.

Remark 3.2. Theorems 3.1 and 3.2 are still valid if the L^∞ norms are changed to L^2 norms. Namely, if $u_0 \in L^2(\Omega)$ and $\|(t^\gamma \partial_t)^k f(\cdot, t)\|_{L^2(\Omega)} \le C_k$ for $k \ge 0$ and $t \in (0, 1]$, then the numerical solution defined in (3.5)–(3.6) has the following error bound for the linear subdiffusion equation:

$$\max_{1\le n\le N} \|u(t_n) - u_n\|_{L^2(\Omega)} \le C_k m^{-k} + Ce^{-\sqrt{M}/C},$$

which holds for all fixed integer $k \ge 1$ and sufficiently large m and M. The proof of this result is the same as the proof of Theorem 3.2 below by changing all the L^∞ norms to L^2 norms.

Proof. We define an auxiliary function u^*, which is the solution of the following linear subdiffusion problem (with the source function replaced by $V_m^r f$):

$$\begin{cases} \partial_t^\alpha u^* - \Delta u^* = V_m^r f & \text{in } \Omega \times (0,1], \\ u^* = 0 & \text{on } \partial\Omega \times (0,1], \\ u^*(0) = u_0 & \text{in } \Omega. \end{cases} \tag{3.9}$$

Then the error $e_n = u(t_n) - u_n$ can be decomposed into $e_n = \tilde{e}_n + e_n^*$, with

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

Since u_n is the quadrature approximation of the contour integral representation of $u^*(t_n)$, i.e., the value after dropping the two remainders in (2.6), the estimates in Lemma 2.1 and the L^∞-stability of the VP means imply that $\|V_m^r f\|_{L^\infty(0,1;L^\infty(\Omega))} \le C\|f\|_{L^\infty(0,1;L^\infty(\Omega))} \le C$ and therefore

$$\|e_n^*\|_{L^\infty(\Omega)} \le Ce^{-\sqrt{M}/C}. \tag{3.10}$$

Since $\tilde{e}_n$ represents the error between the exact solution and the auxiliary function u^* due to the change of the source function from f to $V_m^r f$, by using formula (2.1) we can express $\tilde{e}_n$ as follows:

$$\begin{aligned} \tilde{e}_n &= \int_0^{t_1} E(t_n - s)[f(s) - V_m^r f(s)]\,\mathrm{d}s + \sum_{j=2}^{n} \int_{t_{j-1}}^{t_j} E(t_n - s)[f(s) - V_m^r f(s)]\,\mathrm{d}s \\ &=: \mathcal{E}_{n,1} + \mathcal{E}_{n,2}. \end{aligned} \tag{3.11}$$

The first term on the right-hand side of (3.11) can be estimated by using the boundedness of f and $V_m^r f$, and the estimate $\|E(t-s)\|_{L^\infty(\Omega)\to L^\infty(\Omega)} \le C(t-s)^{\alpha-1}$ as shown in (2.4), i.e.,

$$\|\mathcal{E}_{n,1}\|_{L^\infty(\Omega)} \le C \int_0^{t_1} (t_1 - s)^{\alpha-1} \|f\|_{L^\infty(I_1;L^\infty(\Omega))}\,\mathrm{d}s \le Ct_1^\alpha \|f\|_{L^\infty([0,1];L^\infty(\Omega))}.$$

Since $t_1 = \lambda^{1-N}$ and $N = N_m$ satisfies condition (3.7), it follows that $t_1^\alpha \le m^{-k}$ as $m \to \infty$ for any $k \ge 1$. This proves that

$$\|\mathcal{E}_{n,1}\|_{L^\infty(\Omega)} \le C_k m^{-k} \quad \text{as } m \to \infty. \tag{3.12}$$

The second term on the right-hand side of (3.11) can be estimated by using the following approximation error estimate of the VP means, i.e.,

$$\begin{aligned} \|f - V_m^r f\|_{C([t_{j-1},t_j];L^\infty(\Omega))} &\le C_k (m-r)^{-k} \Big(\frac{t_j - t_{j-1}}{2}\Big)^k \|\partial_t^k f\|_{C([t_{j-1},t_j];L^\infty(\Omega))} \\ &\le C_k m^{-k} \Big(\frac{t_j - t_{j-1}}{2}\Big)^k \|\partial_t^k f\|_{C([t_{j-1},t_j];L^\infty(\Omega))}, \end{aligned} \tag{3.13}$$

which is an immediate consequence of Lemma 2.2 and Lemma 2.3, and a scaling transformation from the standard interval $[-1, 1]$ to the current interval $[t_{j-1}, t_j]$.

The last inequality is due to the fact that $r \le \theta m$ for some fixed $\theta \in (0,1)$. Therefore,

$$\begin{aligned}\|\mathcal{E}_{n,2}\|_{L^\infty(\Omega)} &\le \sum_{j=2}^{n} \int_{t_{j-1}}^{t_j} (t_n - s)^{\alpha-1} \|f - V_m^r f\|_{L^\infty(I_j;L^\infty(\Omega))}\,\mathrm{d}s \\ &\le C_k \sum_{j=2}^{n} m^{-k} \int_{t_{j-1}}^{t_j} (t_n - s)^{\alpha-1} \Big(\frac{t_j - t_{j-1}}{2}\Big)^k \|\partial_s^k f\|_{L^\infty(I_j;L^\infty(\Omega))}\,\mathrm{d}s.\end{aligned} \tag{3.14}$$

The condition in (3.4) implies that $\|\partial_s^k f\|_{L^\infty(I_j;L^\infty(\Omega))} \le C t_{j-1}^{-\gamma k}$ and therefore

$$\begin{aligned}\|\mathcal{E}_{n,2}\|_{L^\infty(\Omega)} &\le C_k \sum_{j=2}^{n} m^{-k} \Big(\frac{t_j - t_{j-1}}{2t_{j-1}^{\gamma}}\Big)^k \int_{t_{j-1}}^{t_j} (t_n - s)^{\alpha-1}\,\mathrm{d}s \\ &\le C_k m^{-k} \sum_{j=2}^{n} \lambda^{[(1-\gamma)+\alpha](j-N)},\end{aligned}$$

where have substituted $t_j = \lambda^{j-N}$ into the last inequality. Since $\lambda > 1$ and $n \le N$, the summation of $\lambda^{[(1-\gamma)+\alpha](j-N)}$ for $j = 2, \ldots, n$ is finite and independent of m. This proves that

$$\|\mathcal{E}_{n,2}\|_{L^\infty(\Omega)} \le C_k m^{-k}. \tag{3.15}$$

Then, substituting the estimates of $\|\mathcal{E}_{n,1}\|_{L^\infty(\Omega)}$ and $\|\mathcal{E}_{n,2}\|_{L^\infty(\Omega)}$ into (3.11), we obtain

$$\|\tilde{e}_n\|_{L^\infty(\Omega)} \le C_k m^{-k} \quad \text{for} \quad 1 \le n \le N. \tag{3.16}$$

The error bound in Theorem 3.2 follows from the two estimates in (3.10) and (3.16). ∎

4. The semilinear problem with rough initial data. In this section, we present the spectral method for the semilinear subdiffusion equation with a rough initial value $u_0 \in L^\infty(\Omega)$. Similarly to the linear problem (as explained at the beginning of Section 3), we can focus on the case $T = 1$ and consider the semilinear subdiffusion equation on the unit time interval $[0,1]$. For the simplicity of presentation, we focus on the case $f(u,x,t) = f(u)$ without loss of generality.

4.1. The spectral collocation method. Differently from the linear problem, we first divide the whole interval $[0,1]$ uniformly into N smaller subintervals $I_n = ((n-1)/N, n/N] = (t_{n-1}, t_n]$, $1 \le n \le N$, and then refine the first subinterval $I_1 = [0, t_1]$ into N_1 smaller subintervals. In particular, for a constant $\lambda > 1$ we define

$$\begin{aligned}&I_{1,1} = [t_0, t_{1,1}] := [0, \lambda^{1-N_1}/N], \\ &I_{1,j} = (t_{1,j-1}, t_{1,j}] := (\lambda^{j-1-N_1}/N, \lambda^{j-N_1}/N] \quad \text{for } j = 2, \ldots, N_1.\end{aligned}$$

The division of the whole interval $[0,1]$ uniformly into N smaller subintervals $I_n = ((n-1)/N, n/N]$, $n = 1, \ldots, N$, is to guarantee the stability of the spectral method on each subinterval with respect to the polynomial interpolation of the nonlinear source function. This will become clear in the error analysis, i.e., the L^∞-norm stability with respect to the polynomial interpolation requires the length of the interval to be sufficiently small. The division of the first subinterval I_1 into N_1 smaller subintervals $I_{1,j}$, $j = 1, \ldots, N_1$, with graded stepsizes locally refined towards $t = 0$ is to resolve the singularity of the nonlinear source function at $t = 0$ (similarly to the linear problem).

On each subinterval $I_{1,n}$, we approximate $f(u)$ by its VP means $V_m^r f(u_m)$, where u_m denotes the numerical solution obtained by using polynomial VP means of degree m on each subinterval. In particular, we denote by $t_{1,n}^{m,1} < t_{1,n}^{m,2} < \cdots < t_{1,n}^{m,m}$ the m zeros of the Jacobi polynomial $J_m^{\alpha,\beta}(t)$ of degree m on the interval $I_{1,n} = (t_{1,n-1}, t_{1,n}]$, $1 \le n \le N_1$, and denote by

$$U_{1,n} = (u_{1,n}^{m,1}, u_{1,n}^{m,2}, \ldots, u_{1,n}^{m,m})^\top$$

the vector which contains the numerical solutions at the discrete time levels $t_{1,n}^{m,i}$, $i = 1, \ldots, m$, determined by the following nonlinear system of equations:

$$U_{1,n} = G_{1,n}(U_{1,n}), \tag{4.1}$$

where $G_{1,n} : L^\infty(\Omega)^m \to L^\infty(\Omega)^m$ is a nonlinear mapping defined by

$$G_{1,n}(U_{1,n}) := (v_{1,n}^{m,1}, v_{1,n}^{m,2}, \ldots, v_{1,n}^{m,m})^\top,$$

with

$$\begin{aligned} v_{1,n}^{m,i} &= \sum_{j=-M}^{M} \omega_j e^{z_j} z_j^{\alpha-1} (z_j^\alpha - (t_{1,n}^{m,i})^\alpha \Delta)^{-1} u_0 \\ &\quad + \sum_{j=-M}^{M} \tilde{\omega}_j (\tilde{z}_j^\alpha - \Delta)^{-1} y_{1,n}^{m,i}(\tilde{z}_j) \quad \text{for } i = 1, \ldots, m, \end{aligned} \tag{4.2}$$

and

$$y_{1,n}^{m,i}(\tilde{z}_j) = e^{\tilde{z}_j (t_{1,n}^{m,i} - t_{1,n-1})} y_{1,n-1}(\tilde{z}_j) + \int_{t_{1,n-1}}^{t_{1,n}^{m,i}} e^{\tilde{z}_j (t_{1,n}^{m,i} - s)} [V_m^r f(u_m)](s) \, \mathrm{d}s. \tag{4.3}$$

If $y_{1,n-1}(\tilde{z}_j)$ is known then we can compute $u_{1,n}^{m,i}$, $i = 1, \ldots, m$ by solving the collocation system (4.1) and then compute $y_{1,n}(z)$ by

$$y_{1,n}(\tilde{z}_j) = e^{\tilde{z}_j (t_{1,n} - t_{1,n-1})} y_{1,n-1}(\tilde{z}_j) + \int_{t_{1,n-1}}^{t_{1,n}} e^{\tilde{z}_j (t_{1,n} - s)} [V_m^r f(u_m)](s) \, \mathrm{d}s. \tag{4.4}$$

Similarly, for each subinterval I_n, $2 \le n \le N$, we denote by $t_n^{m,1} < \cdots < t_n^{m,m}$ the m zeros of Jacobi polynomial $J_m^{\alpha,\beta}(x)$ on I_n, and denote by

$$U_n = (u_n^{m,1}, u_n^{m,2}, \ldots, u_n^{m,m})^\top,$$

the vector which contains the numerical solutions at time levels $t_n^{m,i}$, $i = 1, \ldots, m$, determined by the following nonlinear system of equations:

$$U_n = G_n(U_n), \tag{4.5}$$

where $G_n(U_n) := (v_n^{m,1}, v_n^{m,2}, \ldots, v_n^{m,m})^\top$, with

$$\begin{aligned} v_n^{m,i} &= \sum_{j=-M}^{M} \omega_j e^{z_j} z_j^{\alpha-1} (z_j^\alpha - (t_n^{m,i})^\alpha \Delta)^{-1} u_0 \\ &\quad + \sum_{j=-M}^{M} \tilde{\omega}_j (\tilde{z}_j^\alpha - \Delta)^{-1} y_n^{m,i}(\tilde{z}_j) \quad \text{for } i = 1, \ldots, m, \end{aligned} \tag{4.6}$$

and

$$y_n^{m,i}(\tilde{z}_j) = e^{\tilde{z}_j (t_n^{m,i} - t_{n-1})} y_{n-1}(\tilde{z}_j) + \int_{t_{n-1}}^{t_n^{m,i}} e^{\tilde{z}_j (t_n^{m,i} - s)} [V_m^r f(u_m)](s) \, \mathrm{d}s. \tag{4.7}$$

If $y_{n-1}(\tilde{z}_j)$ is known then we can compute $u_n^{m,i}$, $i = 1, \ldots, m$ by solving collocation system (4.5) and then compute $y_n(z)$ by

$$y_n(\tilde{z}_j) = e^{\tilde{z}_j(t_n - t_{n-1})} y_{1,n-1}(\tilde{z}_j) + \int_{t_{n-1}}^{t_n} e^{\tilde{z}_j(t_n - s)} [V_m^r f(u_m)](s)\, \mathrm{d}s. \tag{4.8}$$

The existence, uniqueness and spectral convergence of the numerical solutions defined by (4.1) and (4.5) are guaranteed by the following theorem.

Theorem 4.1. *Let $u \in C([0,1]; L^2(\Omega)) \cap L^\infty(0,1; L^\infty(\Omega))$ be a bounded mild solution of (1.1) with initial value $u_0 \in L^\infty(\Omega)$ and nonlinear source function $f \in C^\infty(\mathbb{R})$. Let $u_{1,n}^{m,i}$ and $u_n^{m,i}$ be the numerical solutions given by (4.2) and (4.6), respectively. Then there exists a positive constant N_* such that for $N \geq N_*$ and $N_1 = N_1(m)$ satisfying*

$$\lim_{m\to\infty} \frac{N_1(m)}{\log(m)} = \infty, \tag{4.9}$$

the nonlinear systems (4.1) and (4.5) have unique solutions in an L^∞-neighborhood of the mild solution, with the following error bounds:

$$\max_{1\leq n\leq N_1} \max_{1\leq i\leq m} \|u(t_{1,n}^{m,i}) - u_{1,n}^{m,i}\|_{L^\infty(\Omega)} \leq C_k(m^{-k} + e^{-\sqrt{M}/C}), \tag{4.10}$$

$$\max_{2\leq n\leq N} \max_{1\leq i\leq m} \|u(t_n^{m,i}) - u_n^{m,i}\|_{L^\infty(\Omega)} \leq C_k(m^{-k} + e^{-\sqrt{M}/C}), \tag{4.11}$$

which hold for all integer $k \geq 1$ and sufficiently large m and M (larger than some constants which are independent of m).

Remark 4.1. Since all the results are based on the properties of the resolvent operator $(z-\Delta)^{-1}$, which has similar properties under the Dirichlet and periodic boundary conditions, the results in this article can be extended to the periodic bounadry condition.

Remark 4.2. It is mentioned at the beginning of Section 3 that the case $T > 1$ can be solved by dividing the time interval into a number of subintervals. Using the same method together with discrete Gronwall's inequality, the error bound will be multiplied by e^{CT} for long-term computation. The factor e^{CT} usually appears in the error estimates for semilinear parabolic equations and subdiffusion equations. The factor e^{CT} may be removed for the linear subdiffusion equation but requires a closer look at the error analysis by taking account of the regularity behaviour of the mild solution as $t \to 0$. This is not studied in the current paper.

Remark 4.3. For the convenience of illustration, we have focused on the semilinear subdiffusion equation with a Laplacian operator in space. However, the results can be extended to more general elliptic partial differential operators which satisfy the resolved estimate in (2.3), such as second-order elliptic partial differential operators with variable coefficients.

Proof. The roughness of the initial value will generate singularity in the solution and the nonlinear source function at $t = 0$. For a bounded mild solution of the semilinear subdiffusion equation with initial value $u_0 \in L^\infty(\Omega)$, it is shown in [22, inequality (3.8)] that both the solution and the source function exhibit singularities in the form of (1.6). In the next two subsections, we present the proof of Theorem 4.1 based on the regularity estimates in (1.6). For the simplicity of notations, we omit the dependence of the constants C on k in the proof.

4.2. Existence, uniqueness and boundedness of the numerical solution. We denote $L = \|u\|_{L^\infty(0,1;L^\infty(\Omega))}$ and modify the definition of the nonlinear function $f:\mathbb{R}\to\mathbb{R}$ in the region $|\sigma|\geq L+1$ so that $f(\sigma)=0$ for $|\sigma|\geq L+2$. For the simplicity of the notation, we still use f to denote the modified function. This modification make the source function $f:\mathbb{R}\to\mathbb{R}$ globally bounded and Lipschitz continuous, but would not have influence on the numerical solution if it satisfies the following condition:

$$\|u_{1,n}^{m,i}\|_{L^\infty(\Omega)} \leq L+1 \quad \text{and} \quad \|u_n^{m,i}\|_{L^\infty(\Omega)} \leq L+1. \tag{4.12}$$

We shall prove the existence and uniqueness of a numerical solution satisfying this condition (for sufficiently large N and N_1).

The existence and uniqueness of numerical solutions would follow from the contractivity of the map $G_{1,n}: L^\infty(\Omega)^m \to L^\infty(\Omega)^m$. For $V=(v_1,\dots,v_m)\in L^\infty(\Omega)^m$, we denote $f(V)=(f(v_1),\dots,f(v_m))$ and $V_m^r f(V)$ the polynomial on the interval $I_{1,n}$ based on the VP mean of the nodal values $f(v_1),\dots,f(v_m)$. Then

$$\begin{aligned}
&\|G_{1,n}(U)-G_{1,n}(V)\|_{L^\infty(\Omega)^m}\\
&\leq \Big\| \sum_{j=-M}^{M} \tilde\omega_j(\tilde z_j^\alpha-\Delta)^{-1}\int_{t_{1,n-1}}^{t} e^{\tilde z_j(t-s)}V_m^r[f(U)-f(V)]\,\mathrm{d}s\Big\|_{L^\infty(I_{1,n};L^\infty(\Omega))}\\
&\leq \Big\| \sum_{j=-M}^{M} \tilde\omega_j(\tilde z_j^\alpha-\Delta)^{-1}\int_{t_{1,n-1}}^{t} e^{\tilde z_j(t-s)}V_m^r[f(U)-f(V)]\,\mathrm{d}s\\
&\quad -\int_{\Gamma_{\tilde\lambda}}(z^\alpha-\Delta)^{-1}\int_{t_{1,n-1}}^{t} e^{z(t-s)}V_m^r[f(U)-f(V)]\,\mathrm{d}s\,\mathrm{d}z\Big\|_{L^\infty(I_{1,n};L^\infty(\Omega))}\\
&\quad +\Big\|\int_{\Gamma_{\tilde\lambda}}(z^\alpha-\Delta)^{-1}\int_{t_{1,n-1}}^{t} e^{z(t-s)}V_m^r[f(U)-f(V)]\,\mathrm{d}s\,\mathrm{d}z\Big\|_{L^\infty(I_{1,n};L^\infty(\Omega))}\\
&=: \mathcal{F}_1+\mathcal{F}_2.
\end{aligned}$$

$\mathcal{F}_1$ can be estimated by using the L^∞-stability of the VP means and the Lipschitz continuity of the modified function f, i.e., $\|V_m^r[f(U)-f(V)]\|_{L^\infty(I_{1,n};L^\infty(\Omega))}\leq C\|U-V\|_{L^\infty(\Omega)^m}$, and Lemma 2.1, which together imply that

$$\mathcal{F}_1 \leq Ce^{-\sqrt{M}/C}\|U-V\|_{L^\infty(\Omega)^m}. \tag{4.13}$$

$\mathcal{F}_2$ can be converted into the following form:

$$\begin{aligned}
\mathcal{F}_2 &= \Big\|\int_{t_{n-1}}^{t} E(t-s)V_m^r[f(U)-f(V)]\,\mathrm{d}s\Big\|_{L^\infty(I_{1,n};L^\infty(\Omega))}\\
&\leq C\|U-V\|_{L^\infty(\Omega)^m}\int_{t_{n-1}}^{t_n}(t_n-s)^{\alpha-1}\,\mathrm{d}s\\
&= C|I_{1,n}|^\alpha\|U-V\|_{L^\infty(\Omega)^m}.
\end{aligned}\tag{4.14}$$

Since $|I_{1,n}|\leq 1/N$, it follows that

$$\|G_{1,n}(U)-G_{1,n}(V)\|_{L^\infty(\Omega)^m}\leq C(e^{-\sqrt{M}/C}+N^{-\alpha})\|U-V\|_{L^\infty(\Omega)^m}. \tag{4.15}$$

For sufficiently large M and N (bigger than some constants), (4.15) implies that $G_{1,n}: L^\infty(\Omega)^m\to L^\infty(\Omega)^m$ is a contraction and therefore has a unique fixed point, i.e., a numerical solution of (4.1). The existence and uniqueness of a fixed point for the map $G_n: L^\infty(\Omega)^m\to L^\infty(\Omega)^m$, i.e., the existence and uniqueness of a numerical solution of (4.5), can be proved in the same way and therefore omitted.

In the next subsection, we prove that for sufficiently large m, M and N, the numerical solutions $U_{1,n}$ and U_n with the modified source function actually satisfies condition (4.12) and therefore are also the numerical solutions with the original source function. This would prove the existence and uniqueness of numerical solutions with the original source function.

4.3. Error estimation. We define an auxiliary function u^*, which is the solution of the following subdiffusion problem (with the modified source function):

$$\left\{\begin{array}{ll} \partial_t^\alpha u^* - \Delta u^* = V_m^r f(u_m) & \text{in } \Omega\times(0,1],\\ u^*=0 & \text{on } \partial\Omega\times(0,1],\\ u^*(0)=u_0 & \text{in } \Omega. \end{array}\right. \tag{4.16}$$

We also know that the exact solution u satisfies the following equation:

$$\left\{\begin{array}{ll} \partial_t^\alpha u - \Delta u = V_m^r f(u) + \mathcal{E}_f & \text{in } \Omega\times(0,1],\\ u=0 & \text{on } \partial\Omega\times(0,1],\\ u(0)=u_0 & \text{in } \Omega, \end{array}\right. \tag{4.17}$$

where the remainder $\mathcal{E}_f = f(u) - V_m^r f(u)$ satisfies the following estimate for any subinterval $[a,b]\subset(0,1]$:

$$\|\mathcal{E}_f\|_{C([a,b];L^\infty(\Omega))} \le Cm^{-k}\Big(\frac{b-a}{2}\Big)^k \|\partial_t^k f(u)\|_{C([a,b];L^\infty(\Omega))}. \tag{4.18}$$

This is similar to the approximation error bound of VP means for the linear problem; see (3.13). By using expression (2.1) of the solution, the function $\tilde e = u - u^*$ can be written as

$$\tilde e(t) = \int_0^t E(t-s)(V_m^r f(u) - V_m^r f(u_m))\,\mathrm{d}s + \int_0^t E(t-s)\mathcal{E}_f(s)\,\mathrm{d}s. \tag{4.19}$$

Since the modified source function $f:\mathbb{R}\to\mathbb{R}$ is globally bounded and Lipschitz continuous, and the VP means are uniform bounded, it follows that

$$\|V_m^r f(u_m)\|_{L^\infty(I_{1,n};L^\infty(\Omega))} \le C\|f(u_m)\|_{L^\infty(I_{1,n};L^\infty(\Omega))} \le C.$$

Since the numerical solution u_m is the quadrature approximation of the contour integral representation of u^*, it follows from Lemma 2.1 that

$$\|u^* - u_m\|_{L^\infty(I_{1,n};L^\infty(\Omega))} \le Ce^{-\sqrt{M}/C} \quad \text{for } 1\le n\le N_1. \tag{4.20}$$

For $\tilde e_{1,n}^{m,i} = u(t_{1,n}^{m,i}) - u^*(t_{1,n}^{m,i})$, with $1\le i\le m$, $1\le n\le N_1$, setting $t = t_{1,n}^{m,i}$ in (4.19) yields the following estimate:

$$\begin{aligned} \|\tilde e_{1,n}^{m,i}\|_{L^\infty(\Omega)} \le{}& C\int_0^{t_{1,1}} (t_{1,n}^{m,i}-s)^{\alpha-1}\|f(u(s)) - f(u_m)\|_{L^\infty(I_{1,1};L^\infty(\Omega))}\,\mathrm{d}s\\ &+ C\sum_{j=2}^{n-1}\int_{t_{1,j-1}}^{t_{1,j}} (t_{1,n}^{m,i}-s)^{\alpha-1}\max_{1\le i\le m}\|e_{1,j}^{m,i}\|_{L^\infty(\Omega)}\,\mathrm{d}s\\ &+ C\int_{t_{1,n-1}}^{t_{1,n}^{m,i}} (t_{1,n}^{m,i}-s)^{\alpha-1}\max_{1\le i\le m}\|e_{1,n}^{m,i}\|_{L^\infty(\Omega)}\,\mathrm{d}s + Cm^{-k}, \end{aligned}$$

where we have used the result $\|\int_0^{t_{1,n}^{m,i}} E(t_{1,n}^{m,i}-s)\mathcal{E}_f(s)\,\mathrm{d}s\|_{L^\infty(\Omega)} \le Cm^{-k}$, which follows from the same argument as the proof in (3.14)–(3.16) (with $\gamma=1$ therein). Since $\|f(u(s)) - f(u_0)\|_{L^\infty(I_{1,1};L^\infty(\Omega))} \le C$, from the inequality above we obtain

$$\max_{1\le n\le N_1}\max_{1\le i\le m}\|\tilde e_{1,n}^{m,i}\|_{L^\infty(\Omega)} \le Ct_{1,1}^\alpha + Ct_{1,N}^\alpha \max_{1\le n\le N_1}\max_{1\le i\le m}\|e_{1,n}^{m,i}\|_{L^\infty(\Omega)} + Cm^{-k}$$

$$= C\lambda^{(1-N_1)\alpha}N^{-\alpha} + CN^{-\alpha} \max_{1\le n\le N_1}\max_{1\le i\le m}\|e_{1,n}^{m,i}\|_{L^\infty(\Omega)} + Cm^{-k}.$$

Similarly to the proof of (3.12), for sufficiently large N_1 satisfying condition (4.9), we have

$$\max_{1\le n\le N_1}\max_{1\le i\le m}\|\tilde{e}_{1,n}^{m,i}\|_{L^\infty(\Omega)} \le CN^{-\alpha}\max_{1\le n\le N_1}\max_{1\le i\le m}\|e_{1,n}^{m,i}\|_{L^\infty(\Omega)} + Cm^{-k}.$$

Then, substituting (4.20) into the inequality above, we can convert $\tilde{e}_{1,j}^{m,i}$ to $e_{1,j}^{m,i}$ on the left-hand side, i.e.,

$$\begin{aligned}&\max_{1\le n\le N_1}\max_{1\le i\le m}\|e_{1,n}^{m,i}\|_{L^\infty(\Omega)}\\ &\le CN^{-\alpha}\max_{1\le n\le N_1}\max_{1\le i\le m}\|e_{1,n}^{m,i}\|_{L^\infty(\Omega)} + Cm^{-k} + Ce^{-\sqrt{M}/C}.\end{aligned}$$

For sufficiently large N (larger than some constant which is independent of m), the first term on the right-hand side above can be absorbed by the left-hand side. This yields the following error esetimate:

$$\max_{1\le n\le N_1}\max_{1\le i\le m}\|e_{1,n}^{m,i}\|_{L^\infty(\Omega)} \le Cm^{-k} + Ce^{-\sqrt{M}/C}. \tag{4.21}$$

By choosing m and M large enough, we have

$$\max_{1\le n\le N_1}\max_{1\le i\le m}\|e_{1,n}^{m,i}\|_{L^\infty(\Omega)} \le 1$$

and therefore

$$\max_{1\le n\le N_1}\|U_{1,n}\|_{L^\infty(\Omega)^m} \le L+1. \tag{4.22}$$

The same argument can be used to prove that (for sufficiently large m and M)

$$\max_{2\le n\le N}\max_{1\le i\le m}\|e_{n}^{m,i}\|_{L^\infty(\Omega)} \le Cm^{-k} + Ce^{-\sqrt{M}/C}, \tag{4.23}$$

$$\max_{2\le n\le N}\|U_{n}\|_{L^\infty(\Omega)^m} \le L+1. \tag{4.24}$$

This proves that the numerical solution satisfies the constraint in (4.12). Therefore, as we have discussed at the end of Section 4.2, $U_{1,n}$ and U_n are the numerical solutions with the original source function f (which is possibly not globally Lipschitz continuous), satisfying the error bounds in (4.21) and (4.23). This completes the proof of Theorem 4.1. ∎

5. Numerical tests. In this section, we present numerical tests to illustrate spectral convergence of the proposed time discretizations for both linear and semilinear subdiffusion equations with rough initial data. The piecewise linear Galerkin finite element method in space is used with a sufficiently small mesh size that does not affect the observation of the time discretization errors. All the computations are performed by MATLAB R2020b on a personal laptop.

We consider the subdiffusion equation in (1.1) in the domain $\Omega = (0,1)$ up to time $T = 1$, with a discontinuous initial value $u_0 = \chi_{[1/2,1)} \in L^\infty(\Omega)$, where $\chi_{[1/2,1)}$ denotes the characteristic function of the subinterval $[\frac{1}{2},1)$. The parameter λ in the algorithm is chosen to be 2. The number of quadrature points are $2M+1$ with $M = O(m\log^3 m)$, which satisfies the conditions in Theorems 3.1, 3.2 and 4.1. Since the closed form of the exact solution is not known, we compute a reference solution $u_{m_{\mathrm{ref}}}$ with $m_{\mathrm{ref}} = 24$, and compute the errors for $m \le 16$.

The principle of choosing M is to make $e^{-C\sqrt{M}}$ smaller than m^{-k} for all k as $m \to \infty$. Therefore, $M = O(m\log^2 m)$ and $M = O(m\log^3 m)$ both satisfy the requirement theoretically. In the numerical tests we observe that the choice of $M = O(m \log^2 m)$ performs well when m is large, while the choice of $M = O(m \log^3 m)$ performs well for both large m and small m. Therefore, we choose $M = O(m \log^3 m)$ in our numerical experiments below.

5.1. The linear subdiffusion equation. We solve the linear subdiffusion equation with a given source function $f(x,t)$ by the proposed algorithm in Section 3 with $N = \frac{m}{2}$ subintervals. Then the total number of degrees of freedom is $\frac{m^2}{2}$. The errors of the numerical solutions for the smooth source function

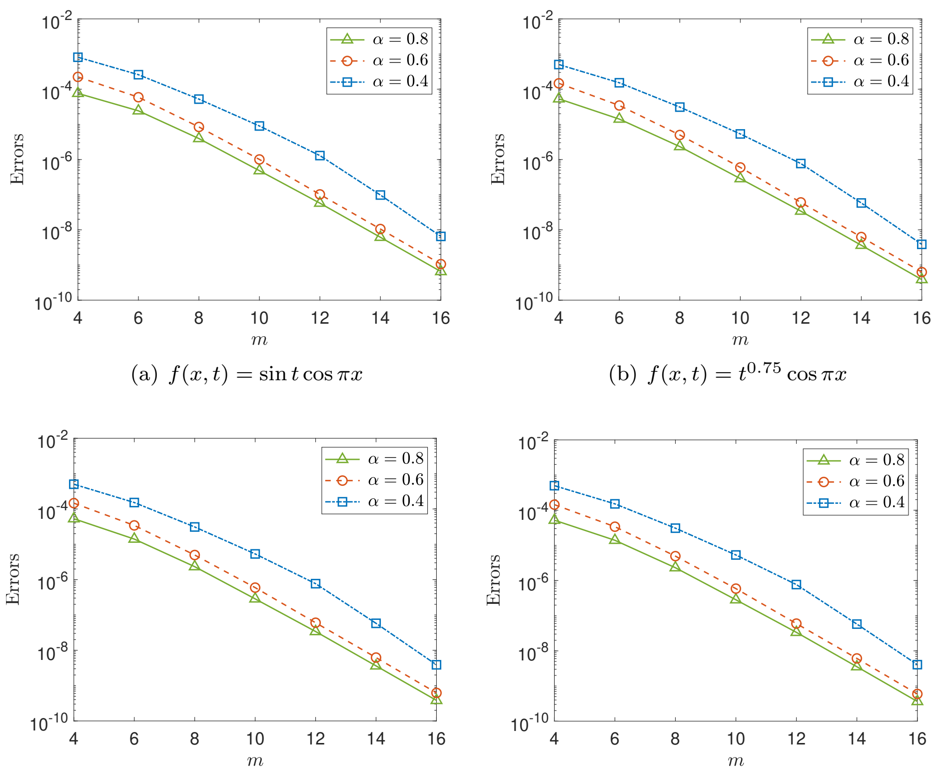
$$f(x,t) = (\sin t) \cos \pi x$$

and the singular source functions

$$f(x,t) = t^\sigma \cos \pi x \quad \text{with } \sigma = 0.75,\ 0.5 \text{ and } 0.25,$$

are presented in Figure 5.1. In particular, the smooth and singular functions satisfy the conditions of Theorems 3.1 and 3.2, respectively.

The numerical results in Figure 5.1 indicate that the proposed method has spectral convergence for the linear subdiffusion equation with both smooth and singular source functions. This is consistent with the theoretical results proved in Theorems 3.1 and 3.2.



(a) $f(x,t) = \sin t \cos \pi x$ (b) $f(x,t) = t^{0.75} \cos \pi x$

(c) $f(x,t) = t^{0.5} \cos \pi x$ (d) $f(x,t) = t^{0.25} \cos \pi x$

Fig. 5.1. *Errors of the numerical solutions for the linear subdiffusion equation*

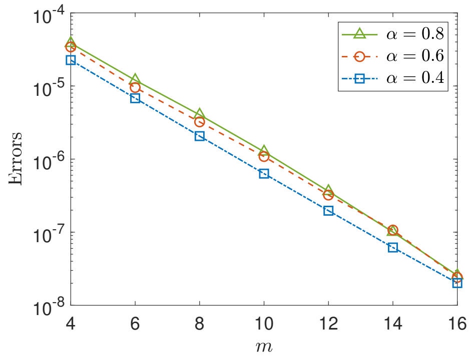


Fig. 5.2. *Errors of the numerical solutions for the semilinear subdiffusion equation*

5.2. The semilinear subdiffusion equation. We consider the semilinear subdiffusion equation in (1.1) with the following nonlinear source function:

$$f(u) = \sin u,$$

which satisfies the condition of Theorem 4.1 and guarantees that the semilinear subdiffusion equation has a unique bounded mild solution. We divide the interval $[0, 1]$ into several subintervals with parameters $N = 1$, $N_1 = \frac{m}{2}$, and total number of degrees of freedom $\frac{m^2}{2}$, and present the errors of the numerical solutions in Figure 5.2 for several different values of $\alpha \in (0, 1)$. The numerical results in Figure 5.2 indicate that the proposed method has spectral convergence for the seimlinear subdiffusion equation with the discontinuous initial value $u_0 = \chi_{[1/2,1)} \in L^\infty(\Omega)$. This is consistent with the theoretical results proved in Theorem 4.1.

6. Conclusions. We have proposed a new spectral method for the linear and semilinear subdiffusion equations in a bounded domain $\Omega \subset \mathbb{R}^d$ under the Dirichlet boundary condition with rough initial data in $L^\infty(\Omega)$ and possibly singular source function by effectively combining several computational techniques, including the contour integral representation of the mild solutions, the quadrature approximation of the contour integrals, the exponential integrator using VP means, and a decomposition of the time interval geometrically refined towards $t = 0$ according to the singularity of the solution and the source function. We have proved the spectral convergence of the proposed method for both linear and semilinear subdiffusion equations with an arbitrary rough initial value $u_0 \in L^\infty(\Omega)$ under the natural regularity of the solutions with strong singularities at $t = 0$ in the form of (1.6).

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