RECOVERY OF THE ORDER OF DERIVATION FOR FRACTIONAL DIFFUSION EQUATIONS IN AN UNKNOWN MEDIUM∗

BANGTI JIN† AND YAVAR KIAN‡

Abstract. In this work, we investigate the recovery of a parameter in a diffusion process given by the order of derivation in time for a class of diffusion type equations, including both classical and time-fractional diffusion equations, from the flux measurement observed at one point on the boundary. The mathematical model for time-fractional diffusion equations involves a Djrbashian-Caputo fractional derivative in time. We prove a uniqueness result in an unknown medium (e.g., diffusion coefficients, obstacle, initial condition and source), i.e., the recovery of the order of derivation in a diffusion process having several pieces of unknown information. The proof relies on the analyticity of the solution at large time, asymptotic decay behavior, strong maximum principle of the elliptic problem and suitable application of the Hopf lemma. Further we provide an easy-to-implement reconstruction algorithm based on a nonlinear least-squares formulation, and several numerical experiments are presented to complement the theoretical analysis.

Key word. order recovery; fractional diffusion; diffusion wave; uniqueness; unknown medium

AMS subject classifications. 35R30, 35R11, 35B30, 65M32

1. Introduction. Let \( \tilde{\Omega} \subset \mathbb{R}^d \) \((d \geq 2)\) be an open bounded and connected subset with a \( C^{1/2,1} \) boundary \( \partial \tilde{\Omega} \) (with \([ \cdot ]\) being the ceiling function), \( \omega \subset \tilde{\Omega} \), and let \( \Omega = \tilde{\Omega} \setminus \omega \). We denote by \( \nu(x) \) the unit outward normal vector to the (outer) boundary \( \partial \tilde{\Omega} \) at a point \( x \in \partial \tilde{\Omega} \), and \( \partial_{\nu} \) the normal derivative. Next we define an elliptic operator \( A \) on the domain \( \Omega \) by

\[
A u(x) := - \sum_{i,j=1}^{d} \partial_{x_i} (a_{i,j}(x) \partial_{x_j} u(x)) + q(x)u(x), \quad x \in \Omega,
\]

where the potential \( q \in C^{1/2,1}(\overline{\Omega}) \) is nonnegative, and the diffusion coefficient matrix \( a := (a_{i,j})_{1 \leq i,j \leq d} \in C^{1 \leq 1/2,1}(\overline{\Omega}; \mathbb{R}^{d \times d}) \) is symmetric and fulfills the following ellipticity condition

\[
\exists c > 0, \quad \sum_{i,j=1}^{d} a_{i,j}(x) \xi_i \xi_j \geq c|\xi|^2, \quad \forall x \in \overline{\Omega}, \forall \xi = (\xi_1, \ldots, \xi_d) \in \mathbb{R}^d.
\]

Let \( \rho \in C^{1/2,1}(\overline{\Omega}) \) obey that for some \( \rho_1 > \rho_0 > 0 \),

\[
0 < \rho_0 \leq \rho(x) \leq \rho_1 < +\infty \quad \text{in } \Omega.
\]

For \( \alpha \in (0, 2) \) and \( 0 < T < +\infty \), consider the following initial boundary value problem for \( u \):

\[
\begin{aligned}
\rho(x) \partial_t^\alpha u + Au &= F, & \text{in } \Omega \times (0, T), \\
u u &= g, & \text{on } \partial \Omega \times (0, T), \\
u u &= 0, & \text{on } \partial \omega \times (0, T), \\
\begin{cases}
\begin{aligned}
u u &= u_0 & \text{if } 0 < \alpha \leq 1, \\
u u &= u_0, & \text{if } 1 < \alpha < 2,
\end{aligned}
\end{cases} & \text{in } \Omega \times \{0\}.
\end{aligned}
\]

∗The work of B.J. is partially supported by UK EPSRC grant EP/T000864/1, and that of Y.K. by the French National Research Agency ANR (project MultiOnde) grant ANR-17-CE40-0029.
†Department of Computer Science, University College London, Gower Street, London WC1E 6BT, UK (b.jin@ucl.ac.uk)
‡Aix Marseille Université, Université de Toulon, CNRS, CPT, Marseille, France (yavar.kian@univ-amu.fr)
In the model (1.4), the notation \( \partial_\alpha^\nu u \) denotes the so-called Djrbashian-Caputo fractional derivative of order \( \alpha \) with respect to \( t \), which, for \( \alpha \in (0,1) \cup (1,2) \), is defined by [23, 39, 12]

\[
\partial_\alpha^\nu u(x,t) := \frac{1}{\Gamma(\alpha - \nu)} \int_0^t (t-s)^{\alpha-1-\nu} \partial_s^\alpha u(x,s) ds, \quad (x,t) \in \Omega \times (0,T),
\]

where the notation \( \Gamma(z) = \int_0^\infty s^{z-1}e^{-s}ds, \Re(z) > 0 \), denotes Euler’s Gamma function, whereas for \( \alpha = 1 \), \( \partial_\alpha^\nu u \) is identified with the usual first order derivative \( \partial_t u \). Throughout we assume that there exists some \( T_1 \in (0,T) \) such that

\[
F(x,t) = 0, \quad (x,t) \in \Omega \times (T_1,T),
\]

\[
g(x,t) = 0, \quad (x,t) \in \partial\Omega \times (T_1,T).
\]

Note that the conditions (1.6)–(1.7) require the source \( F \) and Dirichlet input \( g \) vanish for the time interval \((T_1,T)\). These conditions are needed to ensure the analyticity of the solution \( u(x,t) \) in time \( t \) for any \( t \in (T_1,T) \), and play an essential role in the proof of Theorem 1.1.

The model (1.4), with \( \alpha \neq 1 \), is widely employed to describe anomalous diffusion processes arising in physics, engineering and biology. The cases \( \alpha \in (0,1) \) and \( \alpha \in (1,2) \) are known as subdiffusion and diffusion wave, respectively. The former can be viewed as the macroscopic counterpart of continuous time random walk with a waiting time distribution being heavy tailed (i.e., with a divergent mean) in the sense that the probability density function of the particle appearing at time \( t > 0 \) and spatial location \( x \in \mathbb{R}^d \) satisfies a differential equation of the form (1.4). Subdiffusion has been observed in diffusion in media with fractal geometry [38], transport in column experiments [7] and subsurface flows [1] etc, whereas the diffusion wave case was employed in dynamic viscoelasticity, describing the propagation of mechanical diffusive waves in viscoelastic media which exhibit a power-law creep [34, 35]. We refer interested readers to [37] for physical motivations and many applications.

This paper is concerned with the following inverse problem: to determine the order \( \alpha \) of the fractional derivative \( \partial_\alpha^\nu u(x,t) \) in the model (1.4) from a knowledge of the flux data

\[
h(t) := \partial_\nu u(x_0,t), \quad t \in (T-\delta,T),
\]

for an arbitrary point \( x_0 \in \partial\Omega \) and \( \delta \in (0,T-T_1) \), where \( u \) is a solution to problem (1.4), but without assuming a full knowledge of the problem data (e.g., \( u_0, F, g, \omega, a \) and \( q \)) in the model (1.4). Note that the obstacle \( \omega \) is contained in the domain \( \bar{\Omega} \), and the direct problem (1.4) is posed on the domain \( \Omega = \bar{\Omega} \setminus \omega \) with a boundary \( \partial\Omega = \partial\bar{\Omega} \cup \partial\omega \). We impose a zero Dirichlet boundary condition on \( \partial\omega \) (i.e., solid obstacle), but allow a more general Dirichlet input \( g \) on \( \partial\bar{\Omega} \). The measurement of the flux \( \partial_\nu u(x_0,t) \) at \( x_0 \in \partial\bar{\Omega} \) for the time interval \( t \in (T-\delta,T) \) is performed on the part of the boundary \( \partial\bar{\Omega} \) not intersecting the obstacle \( \omega \), which represents the overposed data for order determination.

The determination of fractional order(s) is probably one of the most natural inverse problems for time-fractional models, as was recently highlighted by the survey [28]; see also [17] for a tutorial on inverse problems for anomalous diffusion. The determination of this parameter allows one to distinguish the type of the concerned diffusion phenomenon, i.e., a classical one (corresponding to the case \( \alpha = 1 \)) or an anomalous one described by a subdiffusive (\( \alpha \in (0,1) \)) or a superdiffusive (\( \alpha \in (1,2) \)) model. For subdiffusion, this inverse problem was first studied by Hatano et al [8], which provided two reconstruction formulas, based on the asymptotics of the solution at small or large time, respectively, and also discussed the numerical recovery for smooth observational data. A first Lipschitz stability result was recently shown in [27]. The work [3] gave a uniqueness result from the terminal measurement. See also [44] for numerical
recovery. Kransnoschok et al [24] studied the recovery of the order in semilinear subdiffusion. There are several works on the simultaneous recovery of the order with the source or other unknowns [9, 10, 30, 33, 18]. We also refer readers to the order recovery in more complex models, e.g., multiple orders [29, 13], spatially-variable order [21], weight in distributed-order [41, 26] and time-variable order [49]. Finally, we mention [45, 46] dealing with similar problems for space-time fractional models and [19] on the simultaneous recovery of the order of derivation with coefficients, a source term and an obstacle.

In this work we consider solutions of problem (1.4) in the following sense.

**Definition 1.1.** A function $u \in W^{[\alpha],1}(0,T;H^{-1}(\Omega)) \cap L^1(0,T;H^1(\Omega))$ is said to be a solution to (1.4) if $u$ solves $\rho(x)\partial_\nu^\alpha u + Au = F$ in the sense of $L^1(0,T;H^{-1}(\Omega))$ and satisfies

$$
\begin{aligned}
&u = g, & &\text{on } \partial \Omega \times (0,T), \\
&u = 0, & &\text{on } \partial \omega \times (0,T), \\
&u = u_0, & &\text{if } 0 \leq \alpha \leq 1, \\
&\partial_t u = 0 & &\text{if } 1 \leq \alpha < 2, \\
&\text{in } \Omega \setminus \{0\}.
\end{aligned}
$$

That is, the governing equation holds in the sense of distribution in $\Omega \times (0,T)$, and the initial and boundary conditions are in the sense of traces of functions $u$ solution to (1.4) if $u$ solves $\rho(x)\partial_\nu^\alpha u + Au = F$ in the sense of $L^1(0,T;H^{-1}(\Omega))$ and satisfies

$$
\begin{aligned}
&u = g, & &\text{on } \partial \Omega \times (0,T), \\
&u = 0, & &\text{on } \partial \omega \times (0,T), \\
&u = u_0, & &\text{if } 0 \leq \alpha \leq 1, \\
&\partial_t u = 0 & &\text{if } 1 \leq \alpha < 2, \\
&\text{in } \Omega \setminus \{0\}.
\end{aligned}
$$

Theorem 1.1. Let $(\alpha_k, \omega_k, a^k, q_k, \rho_k, u^k_0, F_k, g_k)$, $k = 1, 2$, be two admissible tuples, $u^k$, $k = 1, 2$, be the corresponding solution of problem (1.4) on the domain $\Omega_k = \Omega \setminus \omega_k$, and one of the following conditions be fulfilled

(i) $u^k_0 \neq 0$, $k = 1, 2$, is of constant sign.

(ii) $u^k_0 = 0$, for $F^k = \int_0^T F_k(t)dt$ and $g^k = \int_0^T g_k(t)dt$ we have either $g^k_+ \geq 0$ and $F^k_+ \geq 0$ (or $g^k_- \leq 0$ and $F^k_- \leq 0$), $k = 1, 2$. Moreover, $F^k_+ \neq 0$ or $g^k_- \neq 0$, $k = 1, 2$. Then, for any $0 \leq T_1 < T$ and $\delta \in (0,T-T_1)$, we have $u^k \in C([T-\delta,T];C^1(\Omega_k))$, $k = 1, 2$. 

Moreover, for any arbitrarily chosen \( \delta \in (0, T - T_1) \) and \( x_0 \in \partial \Omega \subset \partial \Omega_1 \cap \partial \Omega_2 \), the condition

\[
\partial_{v}u^1(x_0, t) = \partial_{v}u^2(x_0, t), \quad \forall t \in (T - \delta, T)
\]

implies \( \alpha_1 = \alpha_2 \).

The result of Theorem 1.1 is independent of the choice of the problem data \( \omega_k, a^k, q_k, \rho_k, u_0^k, F_k \) and \( g_k, k = 1, 2 \), so long as they satisfy suitable mild assumptions, i.e., condition (1.2)-(1.3), (1.6) / (1.7), and one of the conditions (i), (ii). Thus, Theorem 1.1 still holds even if \( \omega_1 \neq \omega_2, a^1 \neq a^2, q_1 \neq q_2, \rho_1 \neq \rho_2, u_0^1 \neq u_0^2, F_1 \neq F_2 \) and \( g_1 \neq g_2 \), i.e., corresponding to the unique recovery of the fractional order \( \alpha \) in an unknown medium, due to the possibly unknown problem data \( \{ \omega, a, q, \rho, u_0, F, g \} \) in the model (1.4). In addition, we develop an algorithm for recovering the fractional order \( \alpha \) based on a nonlinear least-squares formulation, and illustrate the feasibility of the approach on several one- and two-dimensional numerical tests. The numerical results show that subdiffusion and diffusion wave exhibit distinctly different features for the numerical recovery.

To the best of our knowledge, Theorem 1.1 is the first result on the recovery of the order of derivation for time-fractional models in an unknown medium from a point measurement. It also seems that Theorem 1.1 is the first result of this type stated with a Neumann boundary measurement at an arbitrary point on the boundary of the domain \( \Omega \). Indeed, in all existing results that we are aware of require at least that \( \omega_1 \neq \omega_2 \), \( a^1 \neq a^2 \), \( q_1 \neq q_2 \), \( \rho_1 \neq \rho_2 \), \( u_0^1 \neq u_0^2 \), \( F_1 \neq F_2 \) and \( g_1 \neq g_2 \), i.e., corresponding to the unique recovery of the fractional order \( \alpha \) in an unknown medium, due to the possibly unknown problem data \( \{ \omega, a, q, \rho, u_0, F, g \} \) in the model (1.4). In addition, we develop an algorithm for recovering the fractional order \( \alpha \) based on a nonlinear least-squares formulation, and illustrate the feasibility of the approach on several one- and two-dimensional numerical tests. The numerical results show that subdiffusion and diffusion wave exhibit distinctly different features for the numerical recovery.

The key tools in the analysis include smoothing properties and analyticity in time of the solution \( u \) (or its extension \( \tilde{u} \)) of problem (1.4) for large time; see Propositions 2.2 and 2.3. These properties are derived from a new solution representation, asymptotics of Mittag-Leffler functions and properties of elliptic regularization. The adopted proof techniques allow us to state the main result for a large class of source terms \( F \) and initial conditions \( u_0 \) by only assuming \( F \in L^1(0, T; L^p(\Omega)) \cap W^{1,1}(0, T; L^2(\Omega)) \) and \( u_0 \in L^{2p}(\Omega) \), and moreover treating a nonzero Dirichlet input without imposing any restriction on the space dimension \( d \). To the best of our knowledge, the smoothing effect and the analyticity exhibited in Propositions 2.2 and 2.3 are the first results of this type stated in such a general context and, even for \( F \equiv 0 \) and \( \rho \equiv 0 \), Theorem 1.1 is the first result of this type stated with an initial condition \( u_0 \) lying only in \( L^{2p}(\Omega) \). All existing results that we are aware of require at least that \( u_0 \in H^s(\Omega) \) for some \( s > \frac{d}{2} \) (see e.g. [8, 46]).

The rest of the paper is organized as follows. In Section 2, we present preliminary results, i.e., analyticity and asymptotics of the solution \( u \) to problem (1.4) for an admissible tuple. The proof of Theorem 1.1 is given in Section 3. Several numerical tests are given in Section 4 to illustrate the feasibility of unique order recovery. Throughout, the notation \( C \) denotes a generic positive constant independent of \( t \) and it may change from line to line. Further, we often write a bivariate function \( f(x, t) \) as a vector valued function \( f(t) \), by suppressing the dependence on \( x \). We denote by \( L^2(\Omega; \rho dx) \) the space of measurable functions \( v \) satisfying \( \int_\Omega |v|^2 \rho dx < \infty \) endowed with the inner product \( \langle u, v \rangle_{L^2(\Omega; \rho dx)} = \int_\Omega uv \rho dx \). Note that under condition (1.3), we have \( L^2(\Omega; \rho dx) = L^2(\Omega) \) in the sense of set but equipped with different inner products and norms, which are nonetheless equivalent to each other (under the given condition (1.3) on \( \rho \)), and thus we distinguish only the inner products but not the spaces.
2. Preliminary properties. In this section, we consider the direct problem (1.4) with an admissible tuple \((\alpha, \omega, a, g, \rho, u_0, F, g)\), and show the analyticity and asymptotic behavior of solutions \(u\) of problem (1.4) as \(T \to +\infty\), using the standard separation of variables technique and Mittag-Leffler functions as in [42]. These results will play a central role in the proof of Theorem 1.1 in Section 3.

2.1. Mittag-Leffler function. We shall use extensively the two-parameter Mittag-Leffler function \(E_{\alpha,\beta}(z)\) defined by [23, 39, 12]

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

This function generalizes the exponential function \(e^z\) in that \(E_{1,1}(z) = e^z\), and it is an entire function of order \(\frac{\beta}{\alpha}\) and type 1. It has the following important asymptotic decay behavior in a sector of the complex plane \(\mathbb{C}\) containing the negative real axis; (see [39, pp. 34–35] or [12, Section 3.1] for the proof).

**Lemma 2.1.** Let \(\alpha \in (0, 2), \beta \in \mathbb{R}, \) and \(\mu \in (\frac{\pi}{2}, \min(\pi, \alpha\pi))\). Then for any \(\mu \leq |\arg(z)| \leq \pi\) and \(p \in \mathbb{N}\), there hold

\[
|E_{\alpha,\beta}(z)| \leq c(1 + |z|)^{-\mu},
\]

\[
E_{\alpha,\beta}(z) = -\sum_{k=1}^{p} \frac{z^{-k}}{\Gamma(\beta - k\alpha)} + O(|z|^{-p-1}), \quad \text{as } |z| \to \infty.
\]

In Lemma 2.1 and below, since the set \(\mathbb{Z} \setminus \mathbb{N}\) corresponds to the set of poles of the meromorphic extension to \(\mathbb{C}\) of the Gamma function \(\Gamma(z)\), we use the convention \(\frac{1}{m} = 0, m \in \mathbb{Z} \setminus \mathbb{N}\).

2.2. Analyticity of solutions of problem (1.4). Consider the operator \(A = \rho^{-1}A\) acting on the space \(L^2(\Omega; \rho dx)\) with its domain \(H^2(\Omega) \cap H^1_0(\Omega)\). Then for any \(s > 0\), we may define the fractional power \(A^s\) by spectral decomposition. Let \((\varphi_n)_{n \geq 1}\) be an \(L^2(\Omega; \rho dx)\) orthonormal basis of eigenfunctions of the operator \(A\) associated with the non-decreasing sequence of eigenvalues \((\lambda_n)_{n \geq 1}\) (with multiplicity counted) of \(A\). Then the operator \(A^s\) is defined by

\[
A^sv = \sum_{n=1}^{\infty} \lambda_n^s \langle v, \varphi_n \rangle_{L^2(\Omega; \rho dx)} \varphi_n, \quad \text{with } D(A^s) = \left\{ v \in L^2(\Omega) : \sum_{n=1}^{\infty} \lambda_n^{2s} \langle v, \varphi_n \rangle_{L^2(\Omega; \rho dx)}^2 < \infty \right\},
\]

and the associated graph norm \(\|v\|_{D(A^s)} = (\sum_{n=1}^{\infty} \lambda_n^{2s} \langle v, \varphi_n \rangle_{L^2(\Omega; \rho dx)}^2)^{\frac{1}{2}}\).

Then we have the following result on the analytic extension of the solution \(u\).

**Proposition 2.2.** Let \((\alpha, \omega, a, g, \rho, u_0, F, g)\) be an admissible tuple with \(g \equiv 0\). Then the solution \(u\) of problem (1.4) can be extended to a map \(\tilde{u} \in L^1_{loc}(0, +\infty; L^2(\Omega))\) whose restriction to \(\Omega \times (T_1, +\infty)\) is analytic with respect to \(t \in (T_1, +\infty)\) as a function taking values in \(C^1(\Omega)\).

**Proof.** First, for \(t \in (0, +\infty)\), we define the maps \(u_1\) and \(u_2\) by

\[
u_1(t) = \sum_{n=1}^{\infty} \int_0^{\min(t,T)} (t-s)^{\alpha-1} E_{\alpha,\alpha}(-\lambda_n(t-s)^\alpha) \langle F(s), \varphi_n \rangle_{L^2(\Omega; \rho dx)} ds \varphi_n,
\]

\[
u_2(t) = \sum_{n=1}^{\infty} E_{\alpha,1}(-\lambda_n t^\alpha) \langle u_0, \varphi_n \rangle_{L^2(\Omega; \rho dx)} \varphi_n.
\]

Let \(\tilde{u} = u_1 + u_2\). Then \(\tilde{u} \in L^1_{loc}(0, +\infty; L^2(\Omega))\). Moreover, according to [22, Theorem 2.3], the map \(\tilde{u}\) extends the solution \(u\) to problem (1.4). It remains to show that the restriction of \(u_j\),
Combining this with the estimate \((2.4)\) gives $
abla > 0$, we deduce that, for all $z \in D_{\mu,\pi} := \{ z \in \mathbb{C} : \mu < |\arg(z)| < \pi \}$, we have

$$E_{\alpha,\alpha}(z_1) = -\frac{\ell_1}{\Gamma((1-k)\alpha)} + \mathcal{O}(|z_1|^{-\ell_1-2})$$

$$= -\frac{\ell_1}{\Gamma(-k\alpha)} + \mathcal{O}(|z_1|^{-\ell_1-2}) \quad \text{as } |z_1| \to \infty,$$

since $\frac{1}{\Gamma(0)} = 0$. Therefore, for fixed $\delta > 0$, for all $z_1 \in D_{\mu,\pi}$ with $|z_1| \geq \delta$, we obtain

$$|E_{\alpha,\alpha}(z_1) + \sum_{k=1}^{\ell_1} \frac{z_1^{-k}}{\Gamma(-k\alpha)}| \leq C|z_1|^{-\ell_1-2},$$

with $C > 0$ independent of $z_1$. Note that one can find $\theta_0 \in (0, \min(\frac{(2-\alpha)\pi}{4\alpha}, \frac{\pi}{4}))$ such that for all $s \in (0, T_1)$, $z \in D_{\theta_0}$ and $n \in \mathbb{N}$, we have $-\lambda_n(z - s)^\alpha \in D_{\mu,\pi}$ and $-\lambda_n z^\alpha \in D_{\mu,\pi}$. In addition, for all $r > 0$ and all $\beta \in (-\theta_0, \theta_0)$, we have $|T_1 + \epsilon + r e^{i\beta}| = |T_1 + \epsilon + r \cos \beta|$ and since $0 < \theta_0 < \frac{\pi}{4}$, we deduce $|T_1 + \epsilon + r e^{i\beta}| \geq T_1 + \epsilon + r \cos \theta_0 \geq T_1 + \epsilon$. It follows that for all $z \in D_{\theta_0}$, we have $|z| \geq T_1 + \epsilon$, and thus,

$$| -\lambda_n(z - s)^\alpha| = \lambda_n|z - s|^\alpha \geq \lambda_n|z - s|^\alpha \geq \lambda_1 \epsilon > 0, \quad z \in D_{\theta_0}, \ s \in (0, T_1), \ n \in \mathbb{N}.$$

Therefore, for all $s \in (0, T_1)$, $z \in D_{\theta_0}$ and $n \in \mathbb{N}$, we can apply (2.3) with $z_1 = -\lambda_n(z - s)^\alpha$ and deduce with $C > 0$ independent of $s \in (0, T_1)$, $z \in D_{\theta_0}$ and $n \in \mathbb{N},$

$$|E_{\alpha,\alpha}(-\lambda_n(z - s)^\alpha) + \sum_{k=1}^{\ell_1} \frac{-\lambda_n(z - s)^\alpha(z^{-1} - 1)}{\Gamma(-k\alpha)}| \leq C|\lambda_n(z - s)^\alpha|^{-\ell_1-2}.$$

Multiplying both side of this inequality by $|z - s|^{\alpha-1}$, we obtain

$$\left| (z - s)^{\alpha-1}E_{\alpha,\alpha}(-\lambda_n(z - s)^\alpha) + \sum_{k=1}^{\ell_1} \frac{(-1)^{k+1}(z - s)^{-k\alpha-1}}{\Gamma(-k\alpha)\lambda_n^{k+1}} \right| \leq C\frac{|z - s|^{\alpha-1} - (T_1 + \epsilon)}{|T_1 + \epsilon|^2} \leq C\frac{|z - s|^{\alpha-1} - (T_1 + \epsilon)}{|T_1 + \epsilon|^2} \leq C\frac{|z - s|^{\alpha-1} - (T_1 + \epsilon)}{|T_1 + \epsilon|^2} |z|^{-\gamma}.$$

for all $s \in (0, T_1)$, $z \in D_{\theta_0}$ and $n \in \mathbb{N}$. Note that for all $z \in D_{\theta_0}$, we have $|z| \geq T_1 + \epsilon$. Fixing $\gamma > 0$, we deduce that, for all $z \in D_{\theta_0}$ and $s \in (0, T_1),$

$$|z - s|^{-\gamma} \leq (|z - s|^{-\gamma} \leq (|z - T_1|^{-\gamma} \leq |z|^{-\gamma} \left(1 - \frac{T_1}{|z|}\right)^{-\gamma} \leq \left(1 - \frac{T_1}{|z|}\right)^{-\gamma} |z|^{-\gamma}.$$

Combining this with the estimate (2.4) gives

$$\left| (z - s)^{\alpha-1}E_{\alpha,\alpha}(-\lambda_n(z - s)^\alpha) + \sum_{k=1}^{\ell_1} \frac{(-1)^{k+1}(z - s)^{-k\alpha-1}}{\Gamma(-k\alpha)\lambda_n^{k+1}} \right| \leq C\frac{|z - s|^{\alpha-1} - (T_1 + \epsilon)}{|T_1 + \epsilon|^2 \lambda_n^{\ell_1+2}}.$$
Similarly, by Lemma 2.1, for all $z_1 \in \mathbb{S}_{\mu, \pi}$ with $|z_1| \geq \delta$, we obtain

$$
\left| E_{\alpha,1}(z_1) + \sum_{k=1}^{\ell_1} \frac{z_1^{-k}}{\Gamma(1 - k\alpha)} \right| \leq C|z_1|^{-\ell_1 - 1},
$$

with $C > 0$ independent of $z_1$. For all $z \in D_{\theta_0}$ and $n \in \mathbb{N}$, since $|z| \geq T_1 + \epsilon$, we deduce

$$
| - \lambda_n z^\alpha | = \lambda_n |z|^\alpha \geq \lambda_1 (T_1 + \epsilon)^\alpha > 0.
$$

Therefore, choosing $z_1 = -\lambda_n z^\alpha \in \mathbb{S}_{\mu, \pi}$ and applying the above estimate lead to

$$
E_{\alpha,1}(-\lambda_n z^\alpha) + \sum_{k=1}^{\ell_1} \frac{(-1)^k z^{-k\alpha}}{\Gamma(1 - k\alpha)} \lambda_n^k \leq C \frac{|z|^{-(1+\ell_1)\alpha}}{\lambda_n^{\ell_1 + 1}}.
$$

For all $z \in D_{\theta_0}$ and all $n \in \mathbb{N}$, let

$$
X_n(z) = \int_0^{T_1} (z - s)^{n-1} E_{\alpha,0}(-\lambda_n (z - s)^\alpha) (F(s), \varphi_n)_{L^2(\Omega; \rho \, dx)} \, ds
$$

$$
+ \sum_{k=1}^{\ell_1} \int_0^{T_1} (-1)^k (z - s)^{-k\alpha - 1} v_k(s, \varphi_n)_{L^2(\Omega; \rho \, dx)} \, ds,
$$

$$
Y_n(z) = E_{\alpha,1}(-\lambda_n z^\alpha) \langle u_0, \varphi_n \rangle_{L^2(\Omega; \rho \, dx)} + \sum_{k=1}^{\ell_1} \frac{(-1)^k z^{-k\alpha} w_k}{\Gamma(1 - k\alpha)},
$$

with $v_k = A^{-k-1} F$ and $w_k = A^{-k} u_0$, for $k = 1, \ldots, \ell_1$. One can check that for all $n \in \mathbb{N}$, the maps $X_n$ and $Y_n$ are holomorphic on $D_{\theta_0}$. Moreover, for all $t > T_1 + \epsilon$, we get

$$
u_1(t) + \sum_{k=1}^{\ell_1} \int_0^{T_1} \frac{(-1)^k t^{-k\alpha - 1} v_k(s)}{\Gamma(-k\alpha)} \, ds = \sum_{n=1}^{\infty} X_n(t) \varphi_n,
$$

$$
u_2(t) + \sum_{k=1}^{\ell_1} \frac{(-1)^k t^{-k\alpha} w_k}{\Gamma(1 - k\alpha)} = \sum_{n=1}^{\infty} Y_n(t) \varphi_n.
$$

Under the regularity assumptions on $\Omega$, $a$ and $q$ (from the admissible tuple), the space $D(A^{\ell_1 + 1})$ continuously embeds into $H^{2\ell_1 + 2}(\Omega)$ [6, Theorem 2.5.1.1] and by Sobolev embedding theorem [2], the space $D(A^{\ell_1 + 1})$ embeds continuously into $C^1(\bar{\Omega})$. Therefore, applying (2.5)-(2.6), we deduce that, for all $M, N \in \mathbb{N}$ and all $z \in D_{\theta_0}$,

$$
\left\| \sum_{n=M}^{N} X_n(z) \varphi_n \right\|_{C^1(\bar{\Omega})} \leq C \left\| \sum_{n=M}^{N} X_n(z) \varphi_n \right\|_{D(A^{\ell_1 + 1})}
$$

$$
\leq C |z|^{-(\ell_1 + 1)\alpha} \left\| A^{-\ell_1 - 2} \left( \sum_{n=M}^{N} (F, \varphi_n)_{L^2(\Omega; \rho \, dx)} \varphi_n \right) \right\|_{L^1(0, T; D(A^{\ell_1 + 1}))}
$$

$$
\leq C |z|^{-(\ell_1 + 1)\alpha} \left\| \sum_{n=M}^{N} (F, \varphi_n)_{L^2(\Omega; \rho \, dx)} \varphi_n \right\|_{L^1(0, T; L^2(\Omega; \rho \, dx))},
$$

$$
\left\| \sum_{n=M}^{N} Y_n(z) \varphi_n \right\|_{C^1(\bar{\Omega})} \leq C \left\| \sum_{n=M}^{N} Y_n(z) \varphi_n \right\|_{D(A^{\ell_1 + 1})}.
with $C > 0$ being a constant independent of $M$, $N$ and $z$. The estimates (2.7)-(2.8) imply that, for any compact set $K \subset D_{\theta_0}$, the sequences $\sum_{n=1}^{N} X_n(z)\varphi_n$, $\sum_{n=1}^{N} Y_n(z)\varphi_n$, for $N \in \mathbb{N}$, converge uniformly with respect to $z \in K$ as functions taking values in $C^4(\Omega)$. This proves that the map $u_j^\ast$, $j = 1, 2$, given by $u_j^\ast(t) = \sum_{n=1}^{\infty} X_n(t)\varphi_n$, $u_j^\ast(t) = \sum_{n=1}^{\infty} Y_n(t)\varphi_n$, for $t \in (T_1 + \epsilon, +\infty)$, are analytic as functions taking values in $C^4(\Omega)$. In addition, since $u_0 \in L^2(\Omega)$ and $F \in L^1(0, T; L^p(\Omega))$, we deduce $v_k \in L^1(0, T; W^{p, p}(\Omega))$ and $w_k \in W^{2, 2p}(\Omega)$, $k = 1, \ldots, \ell_1$ [6, Theorem 2.5.1.1]. This, the condition $p > \frac{4}{3}$ and Sobolev embedding theorem give $v_k \in L^1(0, T; C^4(\Omega))$ and $w_k \in C^4(\Omega)$, $k = 1, \ldots, \ell_1$. Therefore, the maps

$$
\begin{align*}
(2.9) & \quad z \mapsto -\frac{1}{\Gamma(-\kappa)} & \quad z \mapsto -\frac{1}{\Gamma(-\kappa)}
\end{align*}
$$

are respectively holomorphic extensions to $D_{\theta_0}$ of the maps $u_1 - u_1^\ast$ and $u_2 - u_2^\ast$ restricted to $t \in (T_1 + \epsilon, +\infty)$ as functions taking values in $C^4(\Omega)$. Thus, both $u_1$ and $u_2$ are analytic with respect to $t \in (T_1 + \epsilon, +\infty)$ as functions taking values in $C^4(\Omega)$. This proves that $\tilde{u}$ is analytic with respect to $t \in (T_1 + \epsilon, +\infty)$ as a function taking values in $C^4(\Omega)$. □

We obtain a similar result for $F \equiv 0$, $u_0 \equiv 0$ but $g \neq 0$.

**Proposition 2.3.** Let $(\alpha, \omega, a, q, \rho, u_0, F, g)$ be an admissible tuple, $u_0 \equiv 0$ and $F \equiv 0$. Then the solution $u$ of problem (1.4) can be extended to a map $\tilde{u} \in L^1_{\text{loc}}(0, +\infty; L^2(\Omega))$ whose restriction to $\Omega \times (T_1, +\infty)$ is analytic with respect to $t \in (T_1, +\infty)$ as a function taking values in $C^4(\Omega)$.

**Proof.** Since the case for $\alpha = 1$ is direct, we consider only the case $\alpha \in (0, 2) \setminus \{1\}$. We introduce the map for $t \in (0, +\infty)$,

$$
(2.9) \quad \tilde{u}(t) = -\frac{1}{\Gamma(-\kappa)} \left( \sum_{n=1}^{\infty} E_{\alpha, \omega}(-\kappa, n, t-s) \langle g(s), \partial_{t^n} \varphi_n \rangle_{L^2(\partial\Omega)} \varphi_n \right) ds,
$$

where $\langle \cdot, \cdot \rangle_{L^2(\partial\Omega)}$ is the standard $L^2(\partial\Omega)$ inner product. Under the given condition on $g$, one can readily check that $\tilde{u} \in L^1_{\text{loc}}(0, +\infty; L^2(\Omega))$ and, in view of [20, Proposition 3.1], there holds $\tilde{u} = u$ on $\Omega \times (0, T)$. Thus, fixing $\epsilon > 0$ arbitrarily chosen, the proposition is proven if we show that $\tilde{u}$ is analytic with respect to $t \in (T_1 + \epsilon, +\infty)$ as a function taking values in $C^4(\Omega)$. Applying (1.7), we find for $t \in (T_1, +\infty)$,

$$
(2.10) \quad \tilde{u}(t) = -\frac{1}{\Gamma(-\kappa)} \left( \sum_{n=1}^{\infty} E_{\alpha, \omega}(-\kappa, n, t-s) \langle g(s), \partial_{t^n} \varphi_n \rangle_{L^2(\partial\Omega)} \varphi_n \right) ds,
$$

where for $x \in \partial\Omega$, the notation

$$
\partial_{t^n} h(x) := \sum_{i,j=1}^{d} a_{i,j}(x) \partial_{x_i} h(x) \nu_i(x)
$$

8
denotes the conormal derivative. For each \( t \in (0, T) \), let \( G(\cdot, t) \) be the solution of

\[
\begin{aligned}
AG(\cdot, t) &= 0, \quad \text{in } \Omega, \\
G(\cdot, t) &= g(\cdot, t), \quad \text{on } \partial \Omega, \\
G(\cdot, t) &= 0, \quad \text{on } \partial \omega.
\end{aligned}
\]

(2.11)

Since \( g \in L^1(0, T; W^{2-\frac{1}{2}, p}(\partial \Omega)) \cap \bigcap_{k=0}^{[\alpha]} W^{[\alpha]-k,1}(0, T; H^{\frac{1}{2}+\frac{1}{p^*}}(\partial \Omega)) \), by the standard elliptic regularity theory, we have \( G \in L^1(0, T; H^2(\Omega)) \cap L^1(0, T; W^{2,p}(\Omega)) \). We fix also \( y_k(\cdot, t) = A^{-k}G(\cdot, t), \ k = 1, \ldots, \ell_1, \)

\[
\langle y_k(t), \varphi_n \rangle_{L^2(\Omega;\rho dx)} = \frac{(g(t), \varphi_n)_{L^2(\Omega;\rho dx)}}{\lambda_n^k} = -\frac{(g(t), \partial_{\nu_n} \varphi_n)_{L^2(\partial \Omega)}}{\lambda_n^{k+1}}, \quad t \in (0, T), \ n \in \mathbb{N}.
\]

The condition \( G \in L^1(0, T; H^2(\Omega)) \) implies that the sequence

\[
\sum_{n=1}^{N} \frac{(g(t), \partial_{\nu_n} \varphi_n)_{L^2(\partial \Omega)}}{\lambda_n} \varphi_n, \quad N \in \mathbb{N}, \ t \in (0, T),
\]

converges in the sense of \( L^1(0, T; L^2(\Omega)) \). For all \( z \in \mathcal{D}_{\theta_0} \) and all \( n \in \mathbb{N} \), let

\[
H_n(z) = -\int_{0}^{T_1} (z-s)^{-\alpha}E_{\alpha,\alpha}(-\lambda_n(z-s)^\alpha)\langle g(s), \partial_{\nu_n} \varphi_n \rangle_{L^2(\partial \Omega)} ds \\
+ \sum_{k=1}^{\ell_1} \int_{0}^{T_1} (-1)^{k+1} (z-s)^{-k\alpha-1} \langle y_k(s), \varphi_n \rangle_{L^2(\Omega;\rho dx)} ds.
\]

Repeating the argument for Proposition 2.2, for all \( M, N \in \mathbb{N} \) and all \( z \in \mathcal{D}_{\theta_0} \), we obtain

(2.12) \[
\left\| \sum_{n=M}^{\infty} H_n(z) \varphi_n \right\|_{C^1(\Omega)} \leq C \| z \|^{-1-(\ell_1+1)\alpha} \left\| \sum_{n=M}^{\infty} \langle G, \varphi_n \rangle_{L^2(\Omega;\rho dx)} \varphi_n \right\|_{L^1(0, T; L^2(\Omega;\rho dx))},
\]

with \( C > 0 \) being a constant independent of \( M, N \) and \( z \). Then, we deduce that the map

\[
u^*(t) := \sum_{n=1}^{\infty} H_n(t) \varphi_n, \quad t \in (T_1 + \epsilon, +\infty)
\]

is analytic as a function taking values in \( C^1(\Omega) \). Similarly, since \( g \in L^1(0, T; W^{2-\frac{1}{2}, p}(\partial \Omega)) \cap \bigcap_{k=0}^{[\alpha]} W^{[\alpha]-k,1}(0, T; H^{\frac{1}{2}+\frac{1}{p^*}}(\partial \Omega)) \), we deduce \( G \in L^1(0, T; W^{2,p}(\Omega)) \) and, furthermore, applying [6, Theorem 2.5.1.1], the condition \( p > \frac{2}{\alpha} \) and Sobolev embedding theorem [2], we obtain \( y_k \in L^1(0, T; W^{4,p}(\Omega)) \) implies \( L^1(0, T; C^1(\Omega)), \ k = 1, \ldots, \ell_1 \). Hence, repeating the argument for Proposition 2.3, we deduce that \( \bar{u} \) is analytic with respect to \( t \in (T_1 + \epsilon, +\infty) \) as a function taking values in \( C^1(\Omega) \).

\[\square\]

2.3. Asymptotic properties of the analytic extension of solutions of problem (1.4). Now we consider the analytic extension \( \bar{u} \in C(T_1, +\infty; C^1(\Omega)) \) of the solution \( u \) of (1.4) in Propositions 2.2 and 2.3. Thus, for any \( x_0 \in \partial \Omega \), the map \( (T_1, +\infty) \ni t \mapsto \partial_{\nu} \bar{u}(x_0, t) \) belongs to \( C(T_1, +\infty) \). Below we study the asymptotic behavior of \( \partial_{\nu} \bar{u}(x_0, t) \) as \( t \to +\infty \), and analyze separately the three cases, i.e., \( F \equiv 0 \) and \( g \equiv 0 \), \( u_0 \equiv 0 \) and \( g \equiv 0 \), and \( u_0 \equiv 0 \) and \( F \equiv 0 \). The next result gives the asymptotic, as \( t \to +\infty \), for \( t \mapsto \partial_{\nu} \bar{u}(x_0, t) \) when \( F \equiv 0 \) and \( g \equiv 0 \).
Proposition 2.4. Let \((\alpha, \omega, a, q, \rho, u_0, F, g)\) be admissible tuple, \(F \equiv 0, g \equiv 0\) and \(x_0 \in \partial \Omega\). If \(\partial_\nu A^{-1}u_0(x_0) \neq 0\), then the extension \(\tilde{u}\) of the solution \(u\) of problem (1.4) defined in Proposition 2.2 satisfies
\[
(2.13) \quad \partial_\nu \tilde{u}(x_0, t) = -\frac{\partial_\nu A^{-1}u_0(x_0)}{\Gamma(1 - \alpha)} t^{-\alpha} + O(t^{-2\alpha}), \quad \text{as } t \to +\infty.
\]

Proof. Applying (2.8) with \(M = 1\) and \(N = \infty\), we deduce that, for all \(t > T_1 + 1\),
\[
\left\| \tilde{u}(t) + \sum_{k=1}^{\ell_1} \frac{(-1)^k t^{-k\alpha} w_k}{\Gamma(1 - k\alpha)} \right\|_{C^1(\Omega)} \leq C t^{-\alpha(\ell_1 + 1)},
\]
with \(C > 0\) independent of \(t\) and \(w_k = A^{-k}u_0, k = 1, \ldots, \ell_1\). It follows that
\[
\partial_\nu \tilde{u}(x_0, t) = -\sum_{k=1}^{\ell_1} \frac{(-1)^k t^{-k\alpha} \partial_\nu w_k(x_0)}{\Gamma(1 - k\alpha)} + O(t^{-\alpha(\ell_1 + 1)}), \quad \text{as } t \to +\infty
\]
which clearly implies (2.13). □

The next result gives the asymptotics of the map \(t \mapsto \partial_\nu \tilde{u}(x_0, t)\) when \(u_0 \equiv 0\) and \(g \equiv 0\).

Proposition 2.5. Let \((\alpha, \omega, a, q, \rho, u_0, F, g)\) be an admissible tuple, \(u_0 \equiv 0, g \equiv 0\) and \(x_0 \in \partial \Omega\), and let
\[
F^* = \int_0^T F(t) dt \in L^p(\Omega) \cap L^2(\Omega).
\]
If \(\partial_\nu A^{-2}F^*(x_0) \neq 0\), then the extension \(\tilde{u}\) of the solution \(u\) of problem (1.4) defined in Proposition 2.2 satisfies
\[
(2.14) \quad \partial_\nu \tilde{u}(x_0, t) = \frac{\partial_\nu A^{-2}F^*(x_0)}{\Gamma(-\alpha)} t^{-1-\alpha} + O(t^{-1-2\alpha}), \quad \text{as } t \to +\infty.
\]

Proof. Applying (2.7) with \(M = 1\) and \(N = \infty\), we deduce that, for all \(t > T_1 + 1\), we have
\[
\left\| \tilde{u}(t) + \sum_{k=1}^{\ell_1} \int_0^{T_1} \frac{(-1)^{k+1}(t-s)^{-k\alpha-1} v_k(s)}{\Gamma(-k\alpha)} ds \right\|_{C^1(\Omega)} \leq C t^{-1-(\ell_1+1)\alpha},
\]
with \(C > 0\) independent of \(t\) and \(v_k = A^{-k-1}F, k = 1, \ldots, \ell_1\). Combining this with the fact that, for all \(k = 1, \ldots, \ell_1, v_k \in L^1(0, T_1; C^1(\Omega))\), we obtain
\[
\partial_\nu \tilde{u}(x_0, t) = \partial_\nu \left( \int_0^{T_1} \frac{(t-s)^{-\alpha-1} v_1(s)}{\Gamma(-\alpha)} ds \right) + O(t^{-1-2\alpha}), \quad \text{as } t \to +\infty.
\]
Further, we have \((t-s)^{-1-\alpha} = t^{-1-\alpha} + O(t^{-1-2\alpha}),\) for \(s \in (0, T_1),\) as \(t \to +\infty\), and hence,
\[
\partial_\nu \tilde{u}(x_0, t) = t^{-1-\alpha} \partial_\nu \left( \int_0^{T_1} \frac{v_1(s)}{\Gamma(-\alpha)} ds \right) + O(t^{-1-2\alpha}), \quad \text{as } t \to +\infty.
\]
Finally, applying (1.6) and noting
\[
\int_0^{T_1} v_1(s) ds = \int_0^{T_1} A^{-2}F(s) ds = A^{-2}F^*;
\]
we obtain (2.14). □
Let \( G^* = \int_0^T G(s) \mathrm{d}s \), with \( G \) solving (2.11). Then \( G^* \in H^2(\Omega) \cap W^{2,p}(\Omega) \) is the unique solution of the boundary value problem

\[
\begin{aligned}
AG^* = 0, & \quad \text{in } \Omega, \\
G^* = g^*, & \quad \text{on } \partial \tilde{\Omega}, \\
G^* = 0, & \quad \text{on } \partial \omega.
\end{aligned}
\]

(2.15)

Combining this with the arguments in Proposition 2.5 and applying estimate (2.12) give the asymptotics, as \( t \to +\infty \), of the map \( t \mapsto \partial_v u(x_0, t) \), when \( u_0 \equiv 0 \) and \( F \equiv 0 \).

**Proposition 2.6.** Let \((\alpha, \omega, a, q, \rho, u_0, F, g)\) be an admissible tuple, \( u_0 \equiv 0 \), \( F \equiv 0 \) and \( x_0 \in \partial \tilde{\Omega}, \) and \( G^* \in H^2(\Omega) \cap W^{2,p}(\Omega) \) solve (2.15). If \( \partial_v A^{-1}G^*(x_0) \neq 0 \), then \( \tilde{u} \) satisfies

\[
\partial_v \tilde{u}(x_0, t) = \frac{\partial_v A^{-1}G^*(x_0)}{\Gamma(-\alpha)} t^{-1-\alpha} + \mathcal{O}(t^{-1-2\alpha}), \quad \text{as } t \to +\infty.
\]

(2.16)

**Remark 2.7.** The proofs of Propositions 2.4–2.6 indicate that one can actually obtain more precise asymptotic expansions including high-order terms. For example, for \( u_0 \in L^{2p}(\Omega), \) \( F \equiv 0 \) and \( g \equiv 0 \), there holds

\[
\partial_v \tilde{u}(x_0, t) = \sum_{k=1}^{\ell_1} \frac{(-1)^k \partial_v A^{-k} u_0(x_0)}{\Gamma(1-k\alpha)} t^{-k\alpha} + \mathcal{O}(t^{-(\ell_1+1)\alpha}), \quad \text{as } t \to +\infty.
\]

Nonetheless, under the conditions of Theorem 1.1, the leading term in the expansion does not vanish, cf. Lemma 3.1, and suffices the proof of Theorem 1.1.

3. **Proof of Theorem 1.1.** In this section, we give the proof of Theorem 1.1. To this end, for \( k = 1, 2 \), we define the operators corresponding to \( A_k = \rho_k^{-1} \hat{A}_k \) acting on \( L^2(\Omega_k; \rho_k \mathrm{d}x) \) with their domain \( D(A_k) = H^1_0(\Omega_k) \cap H^2(\Omega_k) \). Further, for \( k = 1, 2 \), let

\[
v^k = A_k^{-1} u_0^k \quad \text{and} \quad w^k = A_k^{-2} F_k^* + A_k^{-1} G_k^*,
\]

with \( F_k^* = \int_0^T F_k(t) \mathrm{d}t \) (cf. Proposition 2.5) and \( G_k^* \) is defined in (2.15) with \( g^* = g_0^* \) on the domain \( \Omega_k \) (cf. Propositions 2.3 and 2.6). First we give an auxiliary result on \( v^k \) and \( w^k \).

**Lemma 3.1.** The following statements hold.

(i) If condition (i) of Theorem 1.1 holds, then \( v^k \in C^1(\overline{\Omega}_k) \), and for any \( x_0 \in \partial \tilde{\Omega}, \) \( \partial_v v^k(x_0) \neq 0 \).

(ii) If condition (ii) of Theorem 1.1 holds, then \( w^k \in C^1(\overline{\Omega}_k) \), and for any \( x_0 \in \partial \tilde{\Omega}, \) \( \partial_v w^k(x_0) \neq 0 \).

**Proof.** We suppress the subscript \( k \) in the proof. The regularity \( v \in C^1(\overline{\Omega}) \) and \( w \in C^1(\overline{\Omega}) \) follows directly from Sobolev embedding theorem [2] and the elliptic regularity property (see e.g. [6, Theorem 2.5.1.1]). Under condition (i), \( u_0 \) is of constant sign, and we may assume that \( u_0 \leq 0 \). Note that the function \( v \) solves

\[
\begin{aligned}
\mathcal{A} v = \rho u_0, & \quad \text{in } \Omega, \\
v(x) = 0, & \quad \text{on } \partial \Omega.
\end{aligned}
\]

Since \( \mathcal{A} v = \rho u_0 \leq 0 \) in \( \Omega \), \( u_0 \neq 0 \) and \( v|_{\partial \Omega} = 0 \), the strong maximum principle [5, Theorem 3.5] implies \( v(x) < 0 = v(x_0) \), for \( x \in \Omega \), \( x_0 \in \partial \tilde{\Omega} \subset \partial \Omega \). Thus, the Hopf lemma [5, Lemma 3.4] implies \( \partial_v v(x_0) > 0 \) for \( x_0 \in \partial \tilde{\Omega} \). This shows the assertion in (i).
Now we turn to condition (ii). Since $F^*$ and $g^*$ have the same constant sign, we may assume that $F^* \leq 0$ and $g^* \leq 0$. Let $y = A^{-1}F^*$. Then the function $w$ solves

$$
\begin{cases}
Aw = \rho y + \rho G^*, & \text{in } \Omega, \\
\partial_{\nu} w = 0, & \text{on } \partial \Omega.
\end{cases}
$$

Since $F^* \in L^p(\Omega)$, by [6, Theorem 2.4.2.5], there holds $y \in W^{2,p}(\Omega)$ and, since $p > \frac{d}{2}$ by assumption, the Sobolev embedding theorem implies that $y \in C(\overline{\Omega})$. This, the fact $F^* \neq 0$, $F^* \neq 0$ and the maximum principle [5, Corollary 3.2] imply $y \leq 0$. Similarly, we can prove $G^* \leq 0$ and it follows $\max(\rho y, \rho G^*) \leq 0$. Moreover, the fact that $F^* \neq 0$ or $g^* \neq 0$ implies that $ho y \neq 0$ or $\rho G^* \neq 0$. Thus $\rho y + \rho G^* \leq 0$ and $\rho y + \rho G^* \neq 0$. Consequently, by repeating the above application of the strong maximum principle and the Hopf lemma, we deduce that, for all $x_0 \in \partial \Omega$, we have $\partial_{\nu} w(x_0) > 0$.

Now we can give the proof of Theorem 1.1.

**Proof.** Let $u^k$, $k = 1, 2$, be the extension, introduced in Proposition 2.2 and 2.3, of the solution of problem (1.4) corresponding to the admissible tuple $(\alpha_k, \omega_k, a^k, p_k, q_k, u_0^k, F_k, g_k)$. For all $\delta \in (0, T - T_1)$, the regularity $u^k \in C([T - \delta, T]; C^1(\overline{\Omega}))$ is direct from Propositions 2.2 and 2.3. Thus it suffices to show the uniqueness. Fix $\delta \in (0, T - T_1)$, $x_0 \in \partial \Omega$ and let condition (1.8) be fulfilled. From Propositions 2.2 and 2.3, we deduce that $(T_1, +\infty) \ni t \mapsto \partial_{\nu} u^k(x_0, t)$, $k = 1, 2$, is an analytic function. Moreover, following the discussions at the beginning of Proposition 2.2, one can check that the restriction of $u^k$, $k = 1, 2$, to $\Omega \times (0, T)$ coincides with the solution of (1.4) corresponding to the admissible tuple $(\alpha_k, \omega_k, a^k, p_k, q_k, u_0^k, F_k, g_k)$. Therefore, condition (1.8) and unique continuation of analytic functions imply

$$
\partial_{\nu} u^1(x_0, t) = \partial_{\nu} u^2(x_0, t), \quad t \in (T - \delta, +\infty).
$$

It remains to show that the identity (3.1) and one of the conditions (i) and (ii) imply $\alpha_1 = \alpha_2$. First, we prove Theorem 1.1 under condition (i). For $k = 1, 2$, let $(\varphi^k_n)_{n \geq 1}$ be an $L^2(\Omega; \rho_k dx)$ orthonormal basis of eigenfunctions of the operator $A_k$ associated with the non-decreasing sequence of eigenvalues $(\lambda^k_n)_{n \geq 1}$. We recall that $u^k = y_1^k + y_2^k + y_3^k$, with

$$
\begin{align*}
y_1^k(t) &= \sum_{n=1}^{\infty} E_{\alpha,\alpha}(-\lambda^k_n) \langle \varphi^k_n, \varphi^k_n \rangle L^2(\Omega; \rho_k dx) \varphi^k_n, \\
y_2^k(t) &= \sum_{n=1}^{\infty} \int_{0}^{\min(t, T)} (t - s)^{\alpha - 1} E_{\alpha,\alpha}(-\lambda^k_n(t - s)^\alpha) \langle F_k(s), \varphi^k_n \rangle L^2(\Omega; \rho_k dx) ds \varphi^k_n, \\
y_3^k(t) &= -\int_{0}^{\min(t, T)} (t - s)^{\alpha - 1} \left( \sum_{n=1}^{\infty} E_{\alpha,\alpha}(-\lambda^k_n(t - s)^\alpha) \langle g_k(s), \partial_{\nu} \varphi^k_n \rangle L^2(\partial \Omega) \varphi^k_n \right) ds,
\end{align*}
$$

for $t \in (0, +\infty)$. Propositions 2.4, 2.5 and 2.6 yield that for $t \to +\infty$

$$
\begin{align*}
\partial_{\nu} y_1^k(x_0, t) &= -\frac{\partial_{\nu} v^k(x_0)}{\Gamma(1 - \alpha_k)} t^{-\alpha_k} + O(t^{-2\alpha_k}), \\
\partial_{\nu} y_2^k(x_0, t) + \partial_{\nu} y_3^k(x_0, t) &= \frac{\partial_{\nu} u^k(x_0)}{\Gamma(-\alpha_k)} t^{-1 - \alpha_k} + O(t^{-1 - 2\alpha_k}).
\end{align*}
$$

Therefore, we find for $t \to +\infty$,

$$
\partial_{\nu} u^k(x_0, t) = -\frac{\partial_{\nu} v^k(x_0)}{\Gamma(1 - \alpha_k)} t^{-\alpha_k} + O(t^{-\min(2\alpha_k, 1 + \alpha_k)}),
$$

12
and the identity (3.1) implies

\[ -\frac{\partial_t u^1(x_0)}{\Gamma(1 - \alpha_1)} t^{-\alpha_1} + O(t^{-\min(2\alpha_1, 1 + \alpha_1)}) = -\frac{\partial_t u^2(x_0)}{\Gamma(1 - \alpha_2)} t^{-\alpha_2} + O(t^{-\min(2\alpha_2, 1 + \alpha_2)}). \]

Combining this with the fact that \( \partial_t u^k(x_0) \neq 0, k = 1, 2, \) cf. Lemma 3.1(i), one can easily prove by contradiction that (3.2) implies \( \alpha_1 = \alpha_2. \) Note that here for \( \alpha_1 = 1 \) or \( \alpha_2 = 1 \) one can deduce \( \alpha_1 = 1 = \alpha_2, \) since \( \mathbb{Z} \setminus \mathbb{N} \) is the set of poles of \( \Gamma(z) \) in (3.2).

Next, assume that condition (ii) holds. The preceding argumentation gives that for \( t \to +\infty \)

\[ \partial_t u^k(x_0, t) = \frac{\partial_t u^k(x_0)}{\Gamma(-\alpha_k)} t^{-1 - \alpha_k} + O(t^{-1 - 2\alpha_k}). \]

Then, the condition (3.1) implies

\[ \frac{\partial_t u^1(x_0)}{\Gamma(-\alpha_1)} t^{-1 - \alpha_1} + O(t^{-1 - 2\alpha_1}) = \frac{\partial_t u^2(x_0)}{\Gamma(-\alpha_2)} t^{-1 - \alpha_2} + O(t^{-1 - 2\alpha_2}), \quad \text{as } t \to +\infty. \]

This, the fact that \( \partial_t u^k(x_0) \neq 0, k = 1, 2, \) cf. Lemma 3.1(ii), and (3.3) imply that \( \alpha_1 = \alpha_2. \) \( \square \)

**Remark 3.2.** If the inclusion \( \omega = 0, \) the results in Theorem 1.1 hold also for \( d = 1. \)

4. Numerical experiments and discussions. Now we discuss the numerical recovery of the fractional order \( \alpha \) from the flux data \( \partial_t u(x_0, t) \) over the observation window \([T_1, T_2],\) which has not been extensively studied in the literature so far. Hatano et al [7] employed the asymptotic formula and numerical differentiation to recover the order \( \alpha. \) We describe a numerical procedure motivated by the analysis in Section 3. The analysis in Section 3 proceeds in two steps: (i) analytic continuation and (ii) asymptotic matching. The first step can be numerically ill-conditioned, especially when the measurement time horizon \([T_1, T_2] \) is small or \( T_1 \) is very small. Nonetheless, when the observation time \( T_1 \) is sufficiently large, there is a simple recipe to recover the fractional order \( \alpha. \) Specifically, for large \( t, \) when \( u_0 \neq 0, \) the normal derivative \( \partial_t u(x_0, t) \) behaves like

\[ h(t) \equiv \partial_t u(x_0, t) = c_1 t^{-\alpha} + c_2 t^{-2\alpha} + c_3 t^{\alpha - 1} + c_4 t^{1 - 2\alpha} + h.o.t. \]

Thus, one may recover the order \( \alpha \) by fitting to a mixture of powers \( \{t^{-k\alpha}, t^{1-k\alpha}\}_{k=1}^\infty. \) This can be done with the following nonlinear least-squares problem

\[ (\alpha^*, c^*) = \arg \min_{\alpha \in [0, 2]} \sum_{i=1}^N \left( h(t_i) - \sum_{k=1}^K c_k t^{-\alpha_k} \right)^2, \]

with \( \alpha_k = -k\alpha \) or \( \alpha_k = 1 - k\alpha, \) depending on the a priori knowledge on \( u_0 \) (i.e., condition (i) or (ii) / (iii) in Theorem 1.1), \( c = (c_1, \ldots, c_K)^T \in \mathbb{R}^K, \) and \( \{t_i\}_{i=1}^N \) are the sampling points at which discrete observations are available. The formulation (4.2) is very flexible, and capable of handling sparsely / irregularly sparse data points. Note that we do not include a penalty term (e.g., \( \ell^2 \) or \( \ell^1 \)) in the formulation (4.2), since we generally take only a few terms in the expansion (4.1), which has a built-in regularizing effect. In addition, the optimal strength of the penalty should depend on the noise magnitude, which differs dramatically for different cases (e.g., the presence of a nonzero initial condition). Hence the use of a penalty requires much tuning in the current context, and we do not pursue the penalized approach in this work. The optimization problem in (4.2) can be readily solved by any stand-alone optimizer, e.g., limited-memory BFGS. Note that the exponent \( \alpha \) can be warm started by estimating with one single
term (for which the problem can be solved explicitly with log transformation), which can often deliver reasonable estimates. Numerically, we observe that the procedure is fairly robust.

Below we present several numerical tests to show the feasibility of the approach. In all the experiments below, the density $\rho$ is fixed at $\rho \equiv 1$. The exact flux data $h(t) = \partial_t u(x_0,t)$ is generated by solving the direct problem (1.4) over a large time interval $[0, T]$ with $T \gg 1$, which is fixed at $T = 100$ below, discretized with a time step size $\tau = 1 \times 10^{-4}$. The simulation of the direct problem requires extra care in the practical implementation in order to be numerically efficient, since the straightforward implementation of time stepping schemes incur huge time and storage issues. We employ the well known sum of exponentials approximation of the singular kernel to speed up the computation; see the appendix for details. The order $\alpha$ is recovered using eleven discrete observations that are equally spaced within the window $[T_1, T_2]$.

The noisy data $h^\delta$ is generated by adding componentwise noise to the exact data $h(t)$ by $h^\delta(t_i) = h(t_i)(1 + \epsilon \xi(t_i))$, where $\epsilon$ denotes the relative noise level and the noise $\xi(t_i)$ follows the standard Gaussian distribution. Since the subdiffusion and diffusion wave cases exhibit different behavior, we discuss the corresponding numerical results separately.

4.1. Numerical results for subdiffusion. First we present one-dimensional examples, one with nonzero initial condition, and the other two with zero initial condition. The notation $\chi_S$ denotes the characteristic function of a set $S$.

**Example 4.1.** The domain $\Omega$ is taken to be the unit interval $[0, 1]$, and $\omega = \emptyset$. The observation point $x_0$ is the left end point $x_0 = 0$.

(i) $(a, q, u_0, F, g) = (1 + x^2, 1, x^2(1 - x), e^{x(1-x)}x(1 - x)t\chi_{[0,0.1]}(t), 0)$.

(ii) $(a, q, u_0, F, g) = (1, 1 + \sin(x), 0, e^{x^2} \sin(\pi x)\chi_{[0,0.1]}(t), 0)$.

(iii) $(a, q, u_0, F, g) = (1 + \sin(\pi x), \cos(\pi x), 0, 0, e^t \chi_{[0,0.1]}(t))$, with the Dirichlet input $g$ specified on the left end point $x = 0$.

The profiles of the Neumann trace data $h(t) = \partial_t u(x_0,t)$ are shown in Fig. 1 (in the doubly logarithmic scale). Clearly, a power type decay is observed for large $t$ and the decay is faster when the initial condition $u_0$ vanishes identically. This observation agrees well with the theoretical analysis in Section 2, cf. Propositions 2.4–2.6. In particular, it indicates that by fitting fractional powers to the discrete observation points, one may obtain reasonable estimate on the fractional order $\alpha$.

In Table 1 we show the recovered order $\alpha$ for three different observation windows $[T_1, T_2]$, i.e., $[1, 2]$, $[1, 10]$, and $[20, 20]$. The results are obtained using one single term in the least-squares formulation (4.2). It is observed that both observation window $[T_1, T_2]$ and the accuracy of the data influence the quality of order recovery, and the behavior is more or less just as expected: the recovered order $\alpha$ becomes less accurate as the observation window size becomes smaller or
Recovery of the fractional order $\alpha$ for Example 4.1. The blocks (a), (b) and (c) are for the observation window $[1, 2], [1, 10]$ and $[10, 20]$, respectively.

| $\epsilon$\backslash$\alpha$ | (i)  | (ii) | (iii) |
|-----------------------------|------|------|-------|
| $0\%$  | 0.249 | 0.500 | 0.750 |
| (a)  | 0.238 | 0.488 | 0.738 |
| 5$\%$ | 0.185 | 0.435 | 0.685 |
| $0\%$ | 0.249 | 0.500 | 0.750 |
| (b) | 0.244 | 0.494 | 0.744 |
| 5$\%$ | 0.244 | 0.494 | 0.744 |
| $0\%$ | 0.249 | 0.500 | 0.750 |
| (c) | 0.238 | 0.488 | 0.738 |
| 5$\%$ | 0.238 | 0.488 | 0.738 |

Table 1: The numerical results for diffusion wave. Now we present two-dimensional examples for the diffusion wave case. The setting is identical with that of Example 4.2 for subdiffusion, except the fractional order.

Example 4.3. The domain $\Omega = (0, 1)^2$ and the observation point $x_0$ is $(0, 0.5)$.

(i) $(\omega, a, q, u_0, F, g) = (B_{0.2}(0.5, 0.5), 1 + \sin(\pi x_1) x_2(1 - x_2), 1, x_1(1 - x_1)\sin(\pi x_2), x_1(1 - x_1)x_2(1 - x_2)\chi_{[0,0.1]}(t), 0)$.

(ii) $(\omega, a, q, u_0, F, g) = (0, 1, 1, 0, \sin(\pi x_1)x_2^2(1 - x_2)\chi_{[0,0.1]}(t), 0)$.

The numerical results for Example 4.2 are presented in Fig. 2 and Table 2. The decay behavior of the flux $h(t) = \partial_x u(x_0, t)$ is largely comparable with that for Example 4.1: after an initial transient period, which is relatively short, the flux $h(t)$ shows a clearly power type decay, and the decay is faster for cases (ii) and (iii) than case (i), confirming the theoretical predictions from Propositions 2.4–2.6. The accuracy of the recovery is also comparable with the one-dimensional case in Example 4.1. Note that the presence of an obstacle $\omega$ within the domain $\Omega$ does not influence much the recovery accuracy of the order $\alpha$, which agrees with the theoretical analysis.

4.2. Numerical results for diffusion wave. Now we present two-dimensional examples for the diffusion wave case. The setting is identical with that of Example 4.2 for subdiffusion, except the fractional order.

Example 4.3. The domain $\Omega = (0, 1)^2$ and the observation point $x_0$ is $(0, 0.5)$.

(i) $(\omega, a, q, u_0, F, g) = (B_{0.2}(0.5, 0.5), 1 + \sin(\pi x_1) x_2(1 - x_2), 1, x_1(1 - x_1)\sin(\pi x_2), x_1(1 - x_1)x_2(1 - x_2)\chi_{[0,0.1]}(t), 0)$.

(ii) $(\omega, a, q, u_0, F, g) = (0, 1, 1, 0, \sin(\pi x_1)x_2^2(1 - x_2)\chi_{[0,0.1]}(t), 0)$.
Recovery of the fractional order $\alpha$ for Example 4.2. The blocks (a), (b) and (c) are for the observation windows $[1, 2]$, $[1, 10]$ and $[10, 20]$, respectively.

|        | (i) | (ii) | (iii) |
|--------|-----|------|-------|
| $\epsilon$ | 0%  | 1%   | 5%    |
| 0%     | 0.248 | 0.236 | 0.183 |
| 1%     | 0.260 | 0.254 | 0.215 |
| 5%     | 0.260 | 0.254 | 0.215 |
| $\alpha$ | 0.50 | 0.50 | 0.50 |
| 0.75   | 0.879 | 0.867 | 0.814 |
| 0.75   | 0.879 | 0.867 | 0.814 |
| 0.75   | 0.879 | 0.867 | 0.814 |

(iii) $(\omega, a, q, u_0, F, g) = (B_{0.2}(0.5, 0.5), 1 + \sin(\pi x_1)\sin(\pi x_2), 1, 0, 0, x_1(1 - x_1)e^{t\chi_{[0,0.1]}(t)})$, where the Dirichlet boundary condition $g$ is specified only on the bottom boundary $\{(x_1, 0) : 0 \leq x_1 \leq 1\}$, and zero else where.

Fig. 2. The profile of $|h(t)|$ for the three cases of Example 4.2.

The profiles of the Neumann trace $h(t) = \partial_{\nu}u(x_0, t)$ are shown in Fig. 3. Compared with the subdiffusion case, the trace $|h(t)|$ exhibits many more oscillations (or equivalently $h(t)$ oscillates more widely around zero), and as a result, the transient period is much longer. This behavior seems characteristic of the diffusion wave problem: for $\alpha \in (1, 2)$, the Mittag-
Leffler functions \( E_{\alpha,2}(-t) \) and \( E_{\alpha,\alpha}(-t) \) are no longer completely monotone, which is in stark contrast with that for the subdiffusion case (for which both are completely monotone [40, 43] and thus does not change sign). Further, the number of real roots of both functions increases to infinity as the order \( \alpha \) tends to two; see the work [16] for an empirical study on the roots of the function \( E_{\alpha,2}(-t) \). The plots in the middle and right panels show far more oscillations than that in the left most panel (when the \( \alpha \) value is the same). This might be related to the empirical observation that for any fixed \( \alpha \in (1, 2) \), the function \( E_{\alpha,\alpha}(-t) \) has more real roots than \( E_{\alpha,2}(-t) \) (which, however, has not been rigorously proved so far). Note that the magnitude of \( h(t) \) in Case (iii) is very small during the initial time, and thus not displayed in the plot, which differs greatly from the subdiffusion case. In sum, in the diffusion wave case, the boundary data \( h \) does exhibits a power type decay for large time \( t \), but the asymptotic power decay kicks in only for much larger \( t \), which is especially pronounced for the order \( \alpha \) close to two. These observations necessitate measurements at large time so that the least-squares formulation (4.2) is numerically viable.

The numerical recovery results for Example 4.3 are given in Table 3. Just as the plots in Fig. 3 predict, when the initial time \( T_1 \) of the observation window \([T_1, T_2]\) is not sufficient large, the least-squares approach fails to deliver reasonable recovery for large \( \alpha \), as is indicated by notation “–” in the table. This is more dramatic for Cases (ii) and (iii) than Case (i), and it is attributed to the fact when \( T_1 \) is small, the data is still too far away from the asymptotic regime on which the least-squares formulation (4.2) is based. When the initial time \( T_1 \) of the window \([T_1, T_2]\) increases, the recovery becomes viable again and the recovered orders are accurate for data with up to 5% noise, indicating the necessity of large initial observation time \( T_1 \). When the window size decreases from ten to three, the stability of the recovery worsens quite a bit, as confirmed by the numerical results in blocks (b) and (c) in Table 3.

**Appendix A. Numerical schemes for the direct problem (1.4).** In this appendix, we describe the numerical schemes for simulating the direct problem (1.4) for completeness; see the review [15] for further details. For the spatial discretization, we employ the Galerkin finite element method with continuous piecewise linear finite element basis. Let \( X_h \) be the continuous piecewise linear finite element space, subordinated to a shape regular triangulation of the domain \( \Omega \), and \( M_h \) and \( S_h \) be the corresponding mass and stiffness matrices, respectively. The temporal discretization is based on the finite-difference approximation. For any \( N \in \mathbb{N} \) total number of time steps, let \( \tau = \frac{T}{N} \) be the time step size, and \( t_n = n\tau, n = 0, \ldots, N, \)
the time grid. We define the difference approximations (with the shorthand \( u^n = u(t_n) \))
\[
\delta u^{n+\frac{1}{2}} = \tau^{-1}(u^{n+1} - u^n) \text{ and } \delta u^{n+\frac{1}{2}} = \tau^{-1}(\delta u^{n+\frac{1}{2}} - \delta u^{n-\frac{1}{2}}).
\]

Note that a direct implementation of many time stepping schemes suffers from a serious storage issue, due to the nonlocality of the operator \( \partial_t^\alpha u \). Below we describe an implementation based on the sum of exponentials (SOE) approximation of the function \( t^{-\beta} \) over a compact interval \([\delta, T]\) (with \( \delta > 0 \)) [4, 11, 36]. In practice, with proper model reduction, tens of terms suffice a reasonable accuracy.

**Lemma A.1.** For any \( 0 < \beta < 2 \), \( 0 < \delta < 1 \) and \( 0 < \varepsilon < 1 \), there exist \( \{(s_i, \omega_i)\}_{i=1}^{N_\varepsilon} \subset \mathbb{R}_+^2 \) such that \( |t^{-\beta} - \sum_{i=1}^{N_\varepsilon} \omega_i e^{-s_i t}| \leq \varepsilon \), for all \( t \in [\delta, T] \), with \( N_\varepsilon = O((\log \frac{1}{\varepsilon})(\log \log \frac{1}{\varepsilon} + \log \frac{T}{\delta} + (\log \frac{1}{\delta})log \frac{1}{\varepsilon} + \log \frac{1}{\delta})) \).

**A.1. Numerical scheme for subdiffusion** (\( 0 < \alpha < 1 \)). Using piecewise linear interpolation, integration by parts, and the SOE approximation (with \( \beta = 1 + \alpha \) and \( \delta = \tau \)), we can approximate the Djrbashian-Caputo fractional derivative \( \partial_t^\alpha u(t_n) \), \( n \geq 1 \), by
\[
\partial_t^\alpha u^n = \frac{1}{\Gamma(1 - \alpha)} \int_{t_{n-1}}^{t_n} (t_n - s)^{-\alpha} u'(s)ds + \frac{1}{\Gamma(1 - \alpha)} \int_{0}^{t_{n-1}} (t_n - s)^{-\alpha} u'(s)ds
\]
\[
\approx \frac{u^n - u^{n-1}}{\tau^\alpha c_\alpha} + \frac{1}{\Gamma(1 - \alpha)} \left[ \frac{u^{n-1}}{\tau^\alpha} - \frac{u^0}{\tau^\alpha} \alpha \sum_{i=1}^{N_\varepsilon} \omega_i U_{h,i} \right],
\]
with the history terms
\[
U_{h,i}^n = \int_0^{t_{n-1}} e^{-(t_{n-1} - s)} u(s)ds,
\]
and \( c_\alpha = \Gamma(2 - \alpha) \). Since \( u(s) \) is piecewise linear (i.e., \( u(s) = u^{n-2} + \delta_t u^{n-\frac{1}{2}}(s - t_{n-2}) \) over \([t_{n-2}, t_{n-1})\), \( U_{h,i}^n \) satisfies the following recursion
\[
U_{h,i}^n = e^{-s_i \tau} U_{h,i}^{n-1} + \int_{t_{n-2}}^{t_{n-1}} e^{-s_i (t_{n-1} - s)} u(s)ds = e^{-s_i \tau} U_{h,i}^{n-1} + w_i^1 u^{n-1} + w_i^2 u^{n-2},
\]
with the weights
\[
w_i^1 = \frac{e^{-s_i \tau}}{s_i^\alpha} \left( e^{-s_i \tau} - 1 + s_i \tau \right) \text{ and } w_i^2 = \frac{e^{-s_i \tau}}{s_i^\alpha} \left( 1 - e^{-s_i \tau} - e^{-s_i \tau} s_i \tau \right).
\]
When \( s_i \tau \) is very small, the computation of the weights \( w_i^1 \) and \( w_i^2 \) is prone to cancellation errors. Then they may be computed by Taylor expansion as
\[
w_i^1 \approx e^{-s_i \tau} \left( \frac{1}{2} - \frac{s_i \tau}{6} + \frac{(s_i \tau)^2}{24} \right) \text{ and } w_i^2 \approx e^{-s_i \tau} \left( \frac{1}{2} - \frac{s_i \tau}{3} + \frac{(s_i \tau)^2}{8} \right).
\]
The fully discrete scheme reads: with \( U_h^0 = P_h u_0 \) (with \( P_h \) being the \( L^2 \) projection on \( X_h \)), find \( U_h^n \in X_h \) such that for \( n = 1, 2, \ldots, N \),
\[
(M_h + c_\alpha \tau^\alpha S_h) U_h^n = \alpha M_h U_h^{n-1} + (1 - \alpha) M_h \left[ n - \alpha U_h^0 + \alpha \sum_{i=1}^{N_\varepsilon} \omega_i U_{h,i} \right] + c_\alpha \tau^\alpha F_h^n.
\]
This scheme has an accuracy \( O(\tau^{2-\alpha}) \) for smooth solutions [31] and \( O(\tau) \) for general incompatible problem data [14]. The first step may be corrected to be [47]
\[
(M_h + c_\alpha \tau^\alpha S_h) U_h^1 = M_h U_h^0 + c_\alpha \tau^\alpha (F_h^1 + \frac{1}{2} F_h^0 - \frac{1}{2} S_h U_h^0).
\]
Then the overall accuracy of the corrected scheme is \( O(\tau^{2-\alpha}) \) [47].
A.2. Numerical scheme for diffusion wave \((1 < \alpha < 2)\). For \(1 < \alpha < 2\), we employ piecewise quadratic interpolant of \(u\). Let \(H_{2,0}(t)\) be the Hermite quadratic interpolant through \((0, u^0), (\tau, u^1)\) and \((0, u^0)\):

\[
H_{2,0}(t) = u^0 + u^0 t + \tau^{-1}(\delta_t u^\frac{1}{2} - u^0)t^2,
\]

with \(H''_{2,0}(t) = 2\tau^{-1}(\delta_t u^\frac{1}{2} - u'(t_0))\). Next, for any \(u\) defined on the interval \([t_{n-1}, t_{n+1}]\), \(n = 1, \ldots, N - 1\), using \((t_{n-1}, u^{n-1}), (t_{n}, u^{n}), (t_{n+1}, u^{n+1})\), let \(L_{2,n}(t)\) be the quadratic Lagrangian interpolant

\[
L_{2,n}(t) = u^{n-1} + \left(\delta_t u^\frac{n}{2}\right)(t - t_{n-1}) + \frac{1}{2}\left(\delta_t^2 u^n\right)(t - t_{n-1})(t - t_n),
\]

with \(L''_{2,n}(t) = \delta_t^2 u^n\). The scheme employs \(H_{2,0}(t)\) on \([t_0, t_\frac{1}{2}]\) and \(L_{2,n}\) on \([t_{n-\frac{1}{2}}, t_{n+\frac{1}{2}}]\), and SOE approximation (with \(\beta = \alpha - 1\) and \(\delta = \frac{1}{2}\)). Then for \(n = 1\), there holds

\[
\partial_t^\alpha u^\frac{1}{2} = \frac{1}{c_\alpha} \int_0^{t_\frac{1}{2}} (t - s)^{1-\alpha} u''(s)ds \approx \frac{1}{c_\alpha} \int_0^{t_\frac{1}{2}} H''_{2,0}(s)(t - s)^{1-\alpha} ds = \frac{2\alpha^{-1}(u^1 - u^0 - \tau u^0)}{\tau^\alpha c_\alpha},
\]

with \(c_\alpha = \Gamma(2 - \alpha)\) and \(c'_\alpha = \Gamma(3 - \alpha)\). Similarly, for \(n = 2\), we have

\[
\partial_t^\alpha u^\frac{1}{2} = \frac{1}{c_\alpha} \left[ \int_0^{t_\frac{1}{2}} (t - s)^{1-\alpha} u''(s)ds + \int_{t_\frac{1}{2}}^{t_1} (t - s)^{1-\alpha} u''(s)ds \right]
\]

\[\approx \frac{1}{c_\alpha} \left[ \int_0^{t_\frac{1}{2}} H''_{2,0}(s) \sum_{i=1}^N \omega_i e^{-s_i(t_{n-\frac{1}{2}} - s)} ds + \int_{t_\frac{1}{2}}^{t_1} L''_{2,1}(s)(t - s)^{1-\alpha} ds \right]
\]

\[= \frac{1}{c_\alpha} \sum_{i=1}^N \omega_i U_{h,i}^2 + \frac{\delta_t^2 u^1}{c_\alpha} \tau^{2-\alpha} = \frac{1}{c_\alpha} \sum_{i=1}^N \omega_i U_{h,i}^2 + \frac{u^2 - 2u^1 + u_0}{c'_\alpha \tau^\alpha},
\]

with the history term \(U_{h,i}^2\) given by

\[
U_{h,i}^2 = \int_0^{t_\frac{1}{2}} H''_{2,0}(s)e^{-s_i(t_{n-\frac{1}{2}} - s)} ds = \frac{2(\delta_t u^\frac{1}{2} - u^0)}{s_i \tau} e^{-s_i(1 - e^{-\frac{1}{2}s_i \tau})}, \quad i = 1, \ldots, N_e.
\]

For small \(s_i \tau\),

\[
\frac{2(1 - e^{-\frac{1}{2}s_i \tau})}{s_i \tau} \approx 1 - \frac{s_i \tau}{4} + \frac{(s_i \tau)^2}{24}.
\]

Last, for \(n \geq 3\),

\[
\partial_t^\alpha u(t_{n-\frac{1}{2}}) = \frac{1}{c_\alpha} \left[ \int_0^{t_\frac{1}{2}} (t - s)^{1-\alpha} u''(s)ds + \sum_{k=1}^{n-3} \int_{t_k-\frac{1}{2}}^{t_{k+\frac{1}{2}}} (t - s)^{1-\alpha} u''(s)ds \right]
\]

\[\approx \frac{1}{c_\alpha} \left[ \int_0^{t_\frac{1}{2}} H''_{2,0}(s) \sum_{i=1}^N \omega_i e^{-s_i(t_{n-\frac{1}{2}} - s)} ds + \sum_{k=1}^{n-2} \int_{t_{k-\frac{1}{2}}}^{t_{k+\frac{1}{2}}} L''_{2,k}(s) \sum_{i=1}^N \omega_i e^{-s_i(t_{n-\frac{1}{2}} - s)} ds \right.
\]

\[\left. + \int_{t_{n-\frac{1}{2}}}^{t_{n-\frac{1}{2}}} L''_{2,n-1}(s)(t - s)^{1-\alpha} ds \right]
\]

\[= \frac{1}{c_\alpha} \sum_{i=1}^N \omega_i U_{h,i}^2 + \frac{\delta_t^2 u^{n-1}}{c_\alpha} \tau^{2-\alpha} = \frac{1}{c_\alpha} \sum_{i=1}^N \omega_i U_{h,i}^2 + \frac{u^n - 2u^{n-1} + u^{n-2}}{\tau^\alpha c'_\alpha}.\]
where the history term $U_{h,i}^n$ is given by

$$U_{h,i}^n = \int_0^{t_{h,i}} H_{2,0}(s)e^{-s_i(t_{h,i} - s)}\,ds + \sum_{k=1}^{n-2} \int_{t_{k-\frac{1}{2}}}^{t_{k+\frac{1}{2}}} L_{2,k}(s)e^{-s_i(t_{h,i} - s)}\,ds.$$

Note that the history term $U_{h,i}^n$, $n = 3, 4, \ldots$, can be evaluated recursively as

$$U_{h,i}^n = e^{-s_i\tau}U_{h,i}^{n-1} + \delta_i^2 u^{-2} \int_{t_{n-\frac{1}{2}}}^{t_{n+\frac{1}{2}}} e^{-s_i(t_{h,i} - s)}\,ds = e^{-s_i\tau}U_{h,i}^{n-1} + \delta_i^2 u^{-2} \frac{e^{-s_i\tau}}{s_i} (1 - e^{-s_i\tau}).$$

For small $s_i\tau$, the weight

$$\frac{1 - e^{-s_i\tau}}{s_i\tau} \approx 1 - \frac{s_i\tau}{2} + \frac{(s_i\tau)^2}{6} - \frac{(s_i\tau)^3}{24}.$$ 

Then applying the Galerkin finite element method in space, we obtain

$$M_h U^1 + \frac{c_1}{\tau^\alpha} \tau^\alpha S_h U^1 = M_h (U^0 + \tau U^0) - \frac{c'}{\tau^\alpha} \tau^\alpha S_h U^0 + \frac{c'}{\tau^\alpha} \tau^\alpha F_h^1,$$

$$M_h U^n + \frac{c_1}{\tau^\alpha} \tau^\alpha S_h U^n = M_h (2U^{n-1} - U^n - 2) - \frac{c'}{\tau^\alpha} \tau^\alpha S_h U^{n-1} - (2 - \alpha)\tau^\alpha M_h \sum_{i=1}^{N_x} \omega_i U_{h,i}^n$$

$$+ c' \tau^\alpha F_h^{n-\frac{2}{\alpha}}, \quad n = 2, 3, \ldots.$$

This scheme is expected to be $O(\tau)$ accurate for general problem data.

REFERENCES

[1] E. E. Adams and L. W. Gelhar. Field study of dispersion in a heterogeneous aquifer: 2. spatial moments analysis. *Water Res. Research*, 28(12):3293–3307, 1992.

[2] R. A. Adams and J. F. Fournier. *Sobolev Spaces*. Elsevier/Academic Press, Amsterdam, second edition, 2003.

[3] S. Alimov and R. Ashurov. Inverse problem of determining an order of the Caputo time-fractional derivative for a subdiffusion equation. *J. Inverse Ill-Posed Probl.*, 28(5):651–658, 2020.

[4] G. Beylkin and L. Monzón. On approximation of functions by exponential sums. *Appl. Comput. Harmon. Anal.*, 19(1):17–48, 2005.

[5] D. Gilbarg and N. S. Trudinger. *Elliptic Partial Differential Equations of Second Order*. Springer-Verlag, Berlin, revised third edition, 2001.

[6] P. Grisvard. *Elliptic Problems in Nonsmooth Domains*. Pitman, Boston, MA, 1985.

[7] Y. Hatano and N. Hatano. Dispersive transport of ions in column experiments: An explanation of long-tailed profiles. *Water Res. Research*, 34(5):1027–1033, 1998.

[8] Y. Hatano, J. Nakagawa, S. Wang, and M. Yamamoto. Determination of order in fractional diffusion equation. *J. Math-for-Ind.*, 5A:51–57, 2013.

[9] J. Janno. Determination of the order of fractional derivative and a kernel in an inverse problem for a generalized time fractional diffusion equation. *Electron. J. Differential Equations*, pages Paper No. 199, 28, 2016.

[10] J. Janno and N. Kinash. Reconstruction of an order of derivative and a source term in a fractional diffusion equation from final measurements. *Inverse Problems*, 34(2):025007, 19, 2018.

[11] S. Jiang, J. Zhang, Q. Zhang, and Z. Zhang. Fast evaluation of the Caputo fractional derivative and its applications to fractional diffusion equations. *Commun. Comput. Phys.*, 21(3):650–678, 2017.

[12] B. Jin. *Fractional Differential Equations*. Springer, Switzerland, 2021.

[13] B. Jin and Y. Kian. Recovering multiple fractional orders in time-fractional diffusion in an unknown medium. *Proc. A.*, 477(2253):0210468, 21 pp., 2021.

[14] B. Jin, R. Lazarov, and Z. Zhou. An analysis of the L1 scheme for the subdiffusion equation with nonsmooth data. *IMA J. Numer. Anal.*, 36(1):197–221, 2016.

[15] B. Jin, R. Lazarov, and Z. Zhou. Numerical methods for time-fractional evolution equations with non-smooth data: a concise overview. *Comput. Methods Appl. Mech. Engrg.*, 346:332–358, 2019.
[16] B. Jin and W. Rundell. An inverse Sturm-Liouville problem with a fractional derivative. *J. Comput. Phys.*, 231(14):4954–4966, 2012.

[17] B. Jin and W. Rundell. A tutorial on inverse problems for anomalous diffusion processes. *Inverse Problems*, 31(3):035003, 40, 2015.

[18] B. Jin and Z. Zhou. Recovering the potential and order in one-dimensional time-fractional diffusion with unknown initial condition and source. *Inverse Problems*, 37(10):105009, 28 pp., 2021.

[19] Y. Kian. Simultaneous determination of coefficients, internal sources and an obstacle of a diffusion equation from a single measurement. Preprint, arXiv:2007.08947, 2020.

[20] Y. Kian, Z. Li, Y. Liu, and M. Yamamoto. The uniqueness of inverse problems for a fractional equation with a single measurement. *Math. Ann.*, 174:1–31, 2020.

[21] Y. Kian, E. Soccorsi, and M. Yamamoto. On time-fractional diffusion equations with space-dependent variable order. *Ann. Henri Poincaré*, 19(12):3855–3881, 2018.

[22] Y. Kian and M. Yamamoto. Well-posedness for weak and strong solutions of non-homogeneous initial boundary value problems for fractional diffusion equations. *Funct. Calc. Appl. Anal.*, 24(1):168–201, 2021.

[23] A. A. Kilbas, H. M. Srivastava, and J. J. Trujillo. *Theory and Applications of Fractional Differential Equations*. Elsevier Science B.V., Amsterdam, 2006.

[24] M. Krasnoschok, S. Pereverzyev, S. V. Siryk, and N. Vasylyeva. Determination of the fractional order in semilinear subdiffusion equations. *Funct. Calc. Appl. Anal.*, 23(3):694–722, 2020.

[25] A. Kubica, K. Ryszewska, and M. Yamamoto. *Time-Fractional Differential Equations—a Theoretical Approach*. De Gruyter, Berlin, 2019.

[26] Z. Li, K. Fujishiro, and G. Li. Uniqueness in the inversion of distributed orders in ultraslow diffusion equations. *J. Comput. Appl. Math.*, 369:112564, 13, 2020.

[27] Z. Li, X. Huang, and M. Yamamoto. A stability result for the determination of order in time-fractional diffusion equations. *J. Inverse Ill-Posed Probl.*, 28(3):379–388, 2020.

[28] Z. Li, Y. Liu, and M. Yamamoto. Inverse problems of determining parameters of the fractional partial differential equations. In *Handbook of Fractional Calculus with Applications. Vol. 2*, pages 431–442. De Gruyter, Berlin, 2019.

[29] Z. Li and M. Yamamoto. Uniqueness for inverse problems of determining orders of multi-term time-fractional derivatives of diffusion equation. *Appl. Anal.*, 94(3):570–579, 2015.

[30] Z. Li and Z. Zhang. Unique determination of fractional order and source term in a fractional diffusion equation from sparse boundary data. *Inverse Problems*, 36(11):115013, 2020.

[31] Y. Lin and C. Xu. Finite difference/spectral approximations for the time-fractional diffusion equation. *J. Comput. Phys.*, 225(2):1533–1552, 2007.

[32] J. L. Lions and E. Magenes. *Nonhomogeneous Boundary Value Problems and Applications*, volume 2. Springer-Verlag, New York-Heidelberg, 1972.

[33] S. Y. Lukashchuk. Estimation of parameters in fractional subdiffusion equations by the time integral characteristics method. *Comput. Math. Appl.*, 62(3):834–844, 2011.

[34] F. Mainardi. Fractional diffusive waves in viscoelastic solids. In J. L. Wegner and F. R. Norwood, editors, *Nonlinear Waves in Solids*, pages 93–97. ASME/AMR, Fairfield, 1995.

[35] F. Mainardi. *Fractional Calculus and Waves in Linear Viscoelasticity*. Imperial College Press, London, 2010.

[36] W. McLean. Exponential sum approximations for $t^{-\beta}$. In *Contemporary Computational Mathematics—a Celebration of the 80th Birthday of Ian Sloan*. Vol. 1, 2, pages 911–930. Springer, Cham, 2018.

[37] R. Metzler and J. Klafter. The random walk’s guide to anomalous diffusion: a fractional dynamics approach. *Phys. Rep.*, 339(1):77, 2000.

[38] R. R. Nigmatullin. The realization of the generalized transfer equation in a medium with fractal geometry. *Phys. Stat. Sol. B*, 133:425–430, 1986.

[39] I. Podlubny. *Fractional Differential Equations*. Academic Press, Inc., San Diego, CA, 1999.

[40] H. Pollard. The completely monotonic character of the Mittag-Leffler function $E_a(-x)$. *Bull. Amer. Math. Soc.*, 54:1115–1116, 1948.

[41] W. Rundell and Z. Zhang. Fractional diffusion: recovering the distributed fractional derivative from overposed data. *Inverse Problems*, 33(3):035008, 27, 2017.

[42] K. Sakamoto and M. Yamamoto. Initial value/boundary value problems for fractional diffusion-wave equations and applications to some inverse problems. *J. Math. Anal. Appl.*, 382(1):426–447, 2011.

[43] W. R. Schneider. Completely monotone generalized Mittag-Leffler functions. *Exposition. Math.*, 14(1):3–16, 1996.

[44] S. Tatar, R. Tınaztepe, and S. Ulusoy. Simultaneous inversion for the exponents of the fractional time and space derivatives in the space-time fractional diffusion equation. *Appl. Anal.*, 95(1):1–23, 2016.

[45] S. Tatar and S. Ulusoy. A uniqueness result for an inverse problem in a space-time fractional diffusion equation. *Electron. J. Differential Equations*, pages No. 258, 9, 2013.

[46] M. Yamamoto. Uniqueness in determining the orders of time and spatial fractional derivatives. Preprint,
arXiv:2006.15046., 2020.

[47] Y. Yan, M. Khan, and N. J. Ford. An analysis of the modified Li scheme for time-fractional partial differential equations with nonsmooth data. *SIAM J. Numer. Anal.* 56(1):210–227, 2018.

[48] R. Zacher. Weak solutions of abstract evolutionary integro-differential equations in Hilbert spaces. *Funkcial. Ekvac.*, 52(1):1–18, 2009.

[49] X. Zheng, J. Cheng, and H. Wang. Uniqueness of determining the variable fractional order in variable-order time-fractional diffusion equations. *Inverse Problems*, 35(12):125002, 11, 2019.