Regularity theory and numerical algorithm for the fractional Klein-Kramers equation

JING SUN† AND DAXIN NIE‡ AND WEIHUA DENG§

School of Mathematics and Statistics, Gansu Key Laboratory of Applied Mathematics and Complex Systems, Lanzhou University, Lanzhou 730000, P.R. China

[Received on 13 December 2021]

Fractional Klein-Kramers equation can well describe subdiffusion in phase space. In this paper, we develop the fully discrete scheme for fractional Klein-Kramers equation based on the backward Euler convolution quadrature and local discontinuous Galerkin methods. Thanks to the obtained sharp regularity estimates in temporal and spatial directions after overcoming the hypocoercivity of the operator, the complete error analyses of the fully discrete scheme are built. It’s worth mentioning that the convergence of the provided scheme is independent of the temporal regularity of the exact solution. Finally, numerical results are proposed to verify the correctness of the theoretical results.

Keywords: fractional Klein-Kramers equation; regularity estimate; convolution quadrature; local discontinuous Galerkin method; error analysis

1. Introduction

Subdiffusion is ubiquitous in the nature world (see, e.g., Metzler & Klafter, 2000c). Microscopically, it can be modeled by Langevin dynamics with long-tailed trapping (see, e.g., Metzler & Klafter, 2000b). To describe how the presence of the trapping events leads to the macroscopic observation of subdiffusion, the authors establish the fractional Klein-Kramers equation (see, e.g., Metzler & Klafter, 2000a,b). This paper is concerned with the regularity estimate and numerical analysis for the fractional Klein-Kramers equation, i.e.,

\[ \partial_t G(x,v,t) + 0_1^{1-\alpha} \left( \eta v \frac{\partial}{\partial x} - \frac{\gamma}{m} \eta v - \frac{\gamma \eta}{m \beta} \frac{\partial^2}{\partial v^2} \right) G(x,v,t) = 0_1^{1-\alpha} f \quad ((x,v),t) \in \Omega \times (0,T] \]

with initial condition

\[ G(x,v,0) = G_0 \quad (x,v) \in \Omega \]

and boundary conditions

\[ G(x,0,t) = G(x,1,t) = 0 \quad (x,t) \in (0,1) \times (0,T], \]
\[ G(0,v,t) = G(1,v,t) = 0 \quad (v,t) \in (0,1) \times (0,T]. \]

Here \( \Omega = \{ (x,v) \mid 0 < x < 1, 0 < v < 1 \} \); \( T \) denotes the fixed terminal time; \( f \) is source term; \( v \) is the velocity, \( \eta \) is the friction constant, \( m \) is the mass of the particle, \( \gamma \) is the ratio of the intertrapping time.
scale and the internal waiting time scale, and $\beta$ is a variable related to the temperature and Boltzmann’s constant; without loss of generality, we take $\eta = \beta = m = \gamma = 1$ in the following: $0\partial_t^{1-\alpha}G$ is the Riemann-Liouville fractional derivative with $\alpha \in (0, 1)$ defined by (see, e.g., Podlubny, 1999)

$$0\partial_t^{1-\alpha}G = \frac{1}{\Gamma(\alpha)} \frac{\partial}{\partial t} \int_0^t (t - \xi)^{\alpha - 1} G(\xi) d\xi.$$  

(1.3)

In the past few years, there have been some discussions for solving fractional Klein-Kramers equation numerically (see, e.g., Deng & Li, 2011; Gao & Sun, 2012; Li et al., 2012; Nikan et al., 2021). In Deng & Li (2011), the authors consider the finite difference scheme for the fractional Klein-Kramers equation and provide the corresponding error analyses; furthermore the authors use finite difference scheme to solve fractional Klein-Kramers equation with Riesz fractional derivative in Li et al. (2012) and Nikan et al. (2021) provide a hybrid algorithm using the local radial basis functions based on finite difference to obtain the numerical solution of the fractional Klein-Kramers equation. From the above works, it can be noted that the corresponding numerical discussions in Galerkin framework for fractional Klein-Kramers equation are rare.

In this paper, we first build the regularity of Eq. (1.1), and then present the robust numerical scheme and complete error analyses. As for the regularity estimates, to overcome the challenges caused by the hypocoercivity of the operator $\left(\frac{v}{\partial x} - \frac{\partial}{\partial v} r - \frac{\partial^2}{\partial v^2}\right)$, we introduce a new operator $L'$ (one can refer to (2.1)) and provide the corresponding resolvent estimate (see Lemma 2.1); with the help of equivalent form of (1.1) and resolvent estimate, we find

$$\|G(t)\|_{L^2(\Omega)} \leq C\|G_0\|_{L^2(\Omega)} + C\|f(0)\|_{L^2(\Omega)} + C \int_0^t \|f'(s)\|_{L^2(\Omega)} ds$$

and

$$\|G'(t)\|_{L^2(\Omega)} \leq Ct^{-1}\|G_0\|_{L^2(\Omega)} + Ct^{\alpha-1}\|f(0)\|_{L^2(\Omega)} + C \int_0^t (t-s)^{\alpha-1}\|f'(s)\|_{L^2(\Omega)} ds.$$  

Next we use backward Euler convolution quadrature to discretize the temporal derivative and an $O(\tau)$ convergence rate is obtained without any regularity assumptions on the exact solution. At last, we use local discontinuous Galerkin method to discretize spatial derivative; to obtain the stability and the convergence of the fully-discrete scheme, we build a new discrete Grönwall’s inequality (see Lemma 4.1 for the details).

The plan of the paper is as follows. Next, we provide the regularity of the fractional Klein-Kramers equation in temporal and spatial directions, respectively. In Section 3, the time semi-discrete scheme is built by backward Euler convolution quadrature and the resulting error analysis is also provided. Then we use the local discontinuous Galerkin method to discretize the space operator and the error estimate is obtained in Section 4. Section 5 validates the effectiveness of the algorithm by extensive numerical experiments. We conclude the paper with some discussions in the last section. Throughout the paper, $C$ is a positive constant, whose value may differ at different places; $\| \cdot \|$ stands for the operator norm from $L^2(\Omega)$ to $L^2(\Omega)$; and $\overline{\cdot}$ means Laplace transform.

2. Regularity of the solution

Here we first provide some notations, and then present the solution and discuss its regularity. Define $\Gamma_{\theta, \kappa}$ for $\kappa > 0$ and $\theta \in (\frac{\pi}{2}, \pi)$ as

$$\Gamma_{\theta, \kappa} = \{ re^{-i\theta} : r \geq \kappa\} \cup \{ \kappa e^{i\omega} : |\omega| \leq \theta\} \cup \{ re^{i\theta} : r \geq \kappa\},$$

and
As for the operator $L_i$, i.e.,

\[ L_i = \nu \frac{\partial}{\partial x} - \frac{\partial}{\partial v} v - \frac{\partial^2}{\partial v^2} + \frac{1}{2} \]

with boundary conditions (1.2).

Applying $\partial_{\alpha-1}^\alpha$ on both sides of (1.1) and using the definition of $L_i$, we can get the equivalent form of (1.1), i.e.,

\[
\begin{align*}
0 & \partial_{\alpha-1}^\alpha (G(x,v,t) - G_0) + L_i G(x,v,t) = f + \frac{1}{2} G(x,v,t) \\
G(x,v,0) & = G_0 \\
G(x,0,t) & = G(x,1,t) = 0 \\
G(0,v,t) & = 0
\end{align*}
\]

(2.2)

As for the operator $L_i$, according to its definition (2.1) and using integration by parts, it’s easy to check that

\[
(\mathcal{L}G, G) = \int_0^1 v \int_0^1 \frac{\partial}{\partial x} G(x,v,t) dx dv - \frac{1}{2} \int_0^1 \int_0^1 \left( \frac{\partial}{\partial v} (vG(x,v,t)) \right) G(x,v,t) dx dv \\
- \int_0^1 \int_0^1 \frac{\partial^2}{\partial v^2} G(x,v,t) dx dv + \frac{1}{2} \int_0^1 \int_0^1 G(x,v,t) dx dv \\
= \frac{1}{2} \int_0^1 v \int_0^1 \left( \frac{\partial}{\partial x} G(x,v,t) \right)^2 dx dv \\
+ \frac{1}{2} \int_0^1 \int_0^1 \left( \frac{\partial}{\partial v} G(x,v,t) \right)^2 dx dv + \frac{1}{2} \int_0^1 \int_0^1 G(x,v,t) dx dv \\
= \int_0^1 v (1,v,t)'^2 dv - \frac{1}{2} \int_0^1 \int_0^1 v \frac{\partial}{\partial v} (G(x,v,t))^2 dv dx \\
+ \frac{1}{2} \int_0^1 v \frac{\partial}{\partial v} G(x,v,t) dv dx - \frac{1}{2} \int_0^1 \int_0^1 G(x,v,t)^2 dv dx,
\]

where $(\cdot, \cdot)$ means the inner product on $\Omega$. Since $G(x,0,t) = G(x,1,t) = 0$, it follows that

\[
\int_0^1 \int_0^1 v \frac{\partial}{\partial v} G(x,v,t)^2 dv dx = \int_0^1 v G(x,v,t)^2 dx \\
= \int_0^1 v G(x,v,t)^2 dv dx - \int_0^1 G(x,v,t)^2 dx \\
= - \int_0^1 \int_0^1 G(x,v,t)^2 dv dx,
\]

implying

\[
(\mathcal{L}G, G) = \int_0^1 v (1,v,t)^2 dv + \int_0^1 \int_0^1 v \frac{\partial}{\partial v} G(x,v,t) \frac{\partial}{\partial v} G(x,v,t) dv dx \geq 0,
\]

(2.3)
Proof. First, taking inverse Laplace transform for (2.4) leads to
\[ \tilde{G}(z) = E(z)G_0 + \tilde{R}(z)f(0) + \tilde{R}(z)\tilde{f}(z) + \frac{1}{2} \tilde{F}(z)\tilde{G}(z), \] (2.4)
where \( \tilde{\cdot} \) means Laplace transform and
\[ E(z) = z^{\alpha - 1}(z^{\alpha} + \mathcal{L})^{-1}, \]
\[ \tilde{F}(z) = (z^{\alpha} + \mathcal{L})^{-1}, \]
\[ \tilde{R}(z) = z^{-1}(z^{\alpha} + \mathcal{L})^{-1}. \]

Thus, iterating (2.4) \( m (m \in \mathbb{N}) \) times, one can get
\[ \tilde{G}(z) = \sum_{k=0}^{m} \left( \frac{1}{2} \tilde{F}(z) \right)^k (E(z)G_0 + \tilde{R}(z)f(0) + \tilde{R}(z)\tilde{f}(z) + \frac{1}{2} \tilde{F}(z)\tilde{G}(z)). \] (2.5)

Now we present the resolvent estimate of \( \mathcal{L} \).

**Lemma 2.1** Let \( \mathcal{L} \) be defined in (2.1). Then for \( z \in \Sigma_{\theta} = \{ z \in \mathbb{C} : z \neq 0, |\arg z| \leq \theta \} \) with \( \theta \in (\frac{\pi}{2}, \pi) \), there holds
\[ \| (z + \mathcal{L})^{-1} \| \leq C|z|^{-1}. \]

**Proof.** Let \((z + \mathcal{L})u = g\). Then we have
\[ ((z + \mathcal{L})u, u) = (g, u). \]
According to (2.3), one obtains
\[ ((z + \mathcal{L})u, u) \geq z\| u \|_{L^2(\Omega)}^2. \]
Using
\[ (g, u) \leq C\| g \|_{L^2(\Omega)}\| u \|_{L^2(\Omega)} \]
leads to the desired result. \( \square \)

**Remark 2.1** By Lemma 2.1, the inverse Laplace transforms of \( \tilde{E}(z) \), \( \tilde{F}(z) \), and \( \tilde{R}(z) \) satisfy
\[ \| E(t) \| \leq C, \quad \| F(t) \| \leq Ct^{\alpha - 1}, \quad \| R(t) \| \leq Ct^{\alpha}. \] (2.6)

Then we discuss spatial regularity of the solution \( G \).

**Theorem 2.1** Let \( G \) be the solution of (2.2). Assume \( G_0, f(0) \in L^2(\Omega) \), and \( \int_0^1 \| f'(s) \|_{L^2(\Omega)} ds < \infty \). Then one has
\[ \| G(t) \|_{L^2(\Omega)} \leq C\| G_0 \|_{L^2(\Omega)} + C\| f(0) \|_{L^2(\Omega)} + C \int_0^t \| f'(s) \|_{L^2(\Omega)} ds. \]

**Proof.** First, taking inverse Laplace transform for (2.4) leads to
\[ G(t) = E(t)G_0 + \tilde{R}(t)f(0) + \int_0^t \tilde{R}(t-s)f'(s)ds + \frac{1}{2} \int_0^t F(t-s)G(s)ds. \] (2.7)
According to (2.6) and using $T/t \geq 1$, we have

$$\|G(t)\|_{L^2(\Omega)} \leq C \|G_0\|_{L^2(\Omega)} + C \|f(0)\|_{L^2(\Omega)} + C \int_0^t \|f'(s)\|_{L^2(\Omega)} ds + C \int_0^t (t-s)^{\alpha-1} \|G(s)\|_{L^2(\Omega)} ds;$$

By Grönwall’s inequality (see, e.g., Elliott & Larsson, 1992), there exists

$$\|G(t)\|_{L^2(\Omega)} \leq C \|G_0\|_{L^2(\Omega)} + C \|f(0)\|_{L^2(\Omega)} + C \int_0^t \|f'(s)\|_{L^2(\Omega)} ds.$$
Similarly, one can get
\[ I_k \leq C \int_{I_{\beta}} \left| e^{\alpha^2} |z||z|^{-\alpha} |z|^{-1} |dz| \right| \|G_0\|_{L^2(\Omega)} \]
\[ \leq C \|G_0\|_{L^2(\Omega)} \]
\[ \leq C \|G_0\|_{L^2(\Omega)}. \]

Similarly, one can get
\[ III_k \leq C t^{\alpha-1} \left\| f(0) \right\|_{L^2(\Omega)}, \]
\[ IIV_k \leq C \int_0^t (t-s)^{\alpha-1} \left\| f'(s) \right\|_{L^2(\Omega)} ds. \]

As for IV, using \( m = \| t \| \) and Theorem 2.1, we obtain
\[ IV \leq C \int_0^t \int_{I_{\beta}} e^{\alpha^2} |z||z|^{-(m+1)\alpha} |dz| \|G(s)\|_{L^2(\Omega)} ds \]
\[ \leq C \int_0^t (t-s)^{(m+1)\alpha-2} \|G(s)\|_{L^2(\Omega)} ds \]
\[ \leq C \|G_0\|_{L^2(\Omega)} + C \|f(0)\|_{L^2(\Omega)} + C \int_0^t \|f'(s)\|_{L^2(\Omega)} ds. \]

Collecting the above estimates and using \( T/t \geq 1 \) lead to the desired result. \( \square \)

3. Temporal semi-discrete scheme and error analysis

In this section, we consider the temporal semi-discrete scheme of (2.2) and provide the corresponding error estimate. Let \( \tau = T/L (L \in \mathbb{N}^+ \) and \( t_i = i \tau, i = 1, 2, \ldots, L \). Here we use backward Euler convolution quadrature (see, e.g., Lubich, 1988a,b; Lubich et al., 1996) to discretize temporal operator, i.e., the temporal semi-discrete scheme can be written as: Find \( G^n \) such that
\[
\begin{cases}
\sum_{j=0}^{n-1} d_j^{(\alpha)} (G^{n-j} - G_0) + \mathcal{L} G^n = f^n + \frac{1}{2} G^n, \\
G^n(x, 0) = G^n(x, 1) = G^n(0, y) = 0, \\
G^0 = G_0,
\end{cases}
\]
(3.1)

where \( G^n \) is the numerical solution of \( G(x, v, t_n) \), \( f^n = f(t_n) \), and
\[ \sum_{j=0}^{m} d_j^{(\alpha)} \xi^j = (\delta_t(\xi))^{\alpha} = \left( \frac{1 - \xi}{t} \right)^{\alpha}. \]
(3.2)

It’s easy to know that \( d_j^{(\alpha)} \) have the following properties.

Lemma 3.1 (see, e.g., Chen et al., 2009; Deng et al., 2015) Let \( \{d_i^{(\alpha)}\}_{i=0}^\infty \) be defined in (3.2) with \( \alpha \in (0, 1) \). Then we have
\[ d_0^{(\alpha)} > 0; \quad d_i^{(\alpha)} < 0, \quad i \geq 1; \]
\[ \sum_{i=0}^\infty d_i^{(\alpha)} = 0. \]
To obtain the temporal error estimate, we first derive the solution of semi-discrete scheme (3.1). Multiplying $\xi^n$ on both sides of (3.1) and summing $n$ from 1 to $\infty$, we have

$$
\sum_{n=1}^{\infty} \sum_{j=0}^{n-1} d_j^{(\alpha)}(G^{n-j} - G_0)\xi^n + \sum_{n=1}^{\infty} \mathcal{L} G^n \xi^n = \sum_{n=1}^{\infty} f^n \xi^n + \sum_{n=1}^{\infty} \frac{1}{2} G^n \xi^n.
$$

Using the fact $f(t) = f(0) + \int_0^t f'(s)ds$ and introducing $R(t) = \int_0^t f'(s)ds$ lead to

$$
\sum_{n=1}^{\infty} G^n \xi^n = ((\delta t(\xi))^\alpha + \mathcal{L})^{-1} \sum_{n=1}^{\infty} f^0 \xi^n + ((\delta t(\xi))^\alpha + \mathcal{L})^{-1} \sum_{n=1}^{\infty} R(t_n) \xi^n + ((\delta t(\xi))^\alpha + \mathcal{L})^{-1}(\delta t(\xi))^\alpha \sum_{n=1}^{\infty} G^n \xi^n.
$$

Iterating (3.3) $m$ ($m \in \mathbb{N}$) times, one has

$$
\sum_{n=1}^{\infty} G^n \xi^n = \sum_{k=0}^{m} \left( \frac{1}{2} ((\delta t(\xi))^\alpha + \mathcal{L})^{-1} \right)^k ((\delta t(\xi))^\alpha + \mathcal{L})^{-1} \sum_{n=1}^{\infty} f^0 \xi^n + \sum_{k=0}^{m} \left( \frac{1}{2} ((\delta t(\xi))^\alpha + \mathcal{L})^{-1} \right)^k ((\delta t(\xi))^\alpha + \mathcal{L})^{-1} \sum_{n=1}^{\infty} R(t_n) \xi^n + \sum_{k=0}^{m} \left( \frac{1}{2} ((\delta t(\xi))^\alpha + \mathcal{L})^{-1} \right)^k ((\delta t(\xi))^\alpha + \mathcal{L})^{-1}(\delta t(\xi))^\alpha \sum_{n=1}^{\infty} G^n \xi^n.
$$

Thus there holds

$$
G^n = \sum_{k=0}^{m} \frac{1}{2\pi i} \int_{|\xi| = \xi_t} \xi^{-\alpha-1} \left( \frac{1}{2} ((\delta t(\xi))^\alpha + \mathcal{L})^{-1} \right)^k ((\delta t(\xi))^\alpha + \mathcal{L})^{-1} \xi d\xi f(0) + \sum_{k=0}^{m} \frac{1}{2\pi i} \int_{|\xi| = \xi_t} \xi^{-\alpha-1} \left( \frac{1}{2} ((\delta t(\xi))^\alpha + \mathcal{L})^{-1} \right)^k ((\delta t(\xi))^\alpha + \mathcal{L})^{-1} \sum_{j=1}^{\infty} R(t_j) \xi d\xi + \sum_{k=0}^{m} \frac{1}{2\pi i} \int_{|\xi| = \xi_t} \xi^{-\alpha-1} \left( \frac{1}{2} ((\delta t(\xi))^\alpha + \mathcal{L})^{-1} \right)^k ((\delta t(\xi))^\alpha + \mathcal{L})^{-1}(\delta t(\xi))^\alpha G^n \xi d\xi + \frac{1}{2\pi i} \int_{|\xi| = \xi_t} \xi^{-\alpha-1} \left( \frac{1}{2} ((\delta t(\xi))^\alpha + \mathcal{L})^{-1} \right)^{m+1} \sum_{j=1}^{\infty} G^j \xi d\xi.
$$

Taking $\xi_t = e^{-(\kappa+1)\tau}$, using Cauchy’s integral theorem, and introducing $\Gamma^\xi_{\theta,\kappa} = \{z \in \mathbb{C} : \kappa \leq |z| \leq \theta \}$,
According to (2.5), (3.5), and the definition of $\sin$,

$$
G'' = \frac{m}{2\pi i} \int_{\Gamma(x)} e^{\gamma n} \left( \frac{1}{2}((\delta_\tau(e^{-zt}))^\alpha + \mathcal{L})^{-1} \right) \left( (\delta_\tau(e^{-zt}))^\alpha + \mathcal{L} \right)^{-1} \left( 1 - e^{-\tau g} \right) dzf(0)
$$

$$
+ \frac{m}{2\pi i} \int_{\Gamma(x)} e^{\gamma n} \left( \frac{1}{2}((\delta_\tau(e^{-zt}))^\alpha + \mathcal{L})^{-1} \right) \left( (\delta_\tau(e^{-zt}))^\alpha + \mathcal{L} \right)^{-1} \left( \sum_{j=1}^\infty R(t_j)e^{-\tau g}dz \right)
$$

$$
+ \frac{m}{2\pi i} \int_{\Gamma(x)} e^{\gamma n} \left( \frac{1}{2}((\delta_\tau(e^{-zt}))^\alpha + \mathcal{L})^{-1} \right) \left( (\delta_\tau(e^{-zt}))^\alpha + \mathcal{L} \right)^{-1} \left( \sum_{j=1}^\infty G^j e^{-\tau g}dz \right).
$$

(3.5)

**Theorem 3.1** Let $G$ and $G''$ be the solutions of (2.2) and (3.1), respectively. Assume $G_0$, $f(0) \in L^2(\Omega)$, and $\int_0^t (t-s)^{n-1} \|f'(s)\|_{L^2(\Omega)} ds < \infty$. Then one has

$$
\|G(t_n) - G''\|_{L^2(\Omega)} \leq C \tau \left( t_n^{-1} \ln(n) \|G_0\|_{L^2(\Omega)} + t_n^{n-1} \|f(0)\|_{L^2(\Omega)} + \int_0^{t_n} (t_n-s)^{n-1} \|f'(s)\|_{L^2(\Omega)} ds \right).
$$

**Proof.** According to (2.5), (3.5), and the definition of $R(t)$, there exists

$$
\|G(t_n) - G''\|_{L^2(\Omega)} \leq C \sum_{k=0}^m \left\| \int_{\Gamma(x)} e^{\gamma n} \left( \frac{1}{2}(z^\alpha + \mathcal{L})^{-1} \right) \left( z^\alpha + \mathcal{L} \right)^{-1} z^\alpha dzf(0) \right\|_{L^2(\Omega)}
$$

$$
+ C \sum_{k=0}^m \left\| \int_{\Gamma(x)} e^{\gamma n} \left( \frac{1}{2}(z^\alpha + \mathcal{L})^{-1} \right) \left( z^\alpha + \mathcal{L} \right)^{-1} \left( \sum_{j=1}^\infty R(t_j)e^{-\tau g}dz \right) \right\|_{L^2(\Omega)}
$$

$$
+ C \sum_{k=0}^m \left\| \int_{\Gamma(x)} e^{\gamma n} \left( \frac{1}{2}(z^\alpha + \mathcal{L})^{-1} \right) \left( z^\alpha + \mathcal{L} \right)^{-1} G^j dz \right\|_{L^2(\Omega)}
$$

$$
+ C \left\| \frac{1}{2\pi i} \int_{\Gamma(x)} e^{\gamma n} \left( \frac{1}{2}(z^\alpha + \mathcal{L})^{-1} \right) m+1 \tilde{G}dz - \frac{1}{2\pi i} \int_{\Gamma(x)} e^{\gamma n} \left( \frac{1}{2}(z^\alpha + \mathcal{L})^{-1} \right) m+1 \sum_{j=1}^\infty G^j e^{-\tau g}dz \right\|_{L^2(\Omega)}
$$

$$
\leq \sum_{k=0}^m I_k + \sum_{k=0}^m H_k + \sum_{k=0}^m I_k + IV.
$$
For $I_k$, it can be split into three parts, i.e.,

$$I_k \leq C \left\| \int_{f_{\theta,k}^{-1}} e^{\tau_n} \left( \frac{1}{2} (z^\alpha + \mathcal{L})^{-1} \right)^k (z^\alpha + \mathcal{L})^{-1} z^{-1} dz \right\| \| f(0) \|_{L^2(\Omega)}$$

$$+ C \left\| \int_{f_{\theta,k}^{-1}} (e^{\tau_n} - e^{\tau_{n-1}}) \left( \frac{1}{2} (z^\alpha + \mathcal{L})^{-1} \right)^k (z^\alpha + \mathcal{L})^{-1} z^{-1} dz \right\| \| f(0) \|_{L^2(\Omega)}$$

$$+ C \left\| \int_{f_{\theta,k}^{-1}} e^{\tau_{n-1}} \left( \frac{1}{2} (z^\alpha + \mathcal{L})^{-1} \right)^k (z^\alpha + \mathcal{L})^{-1} z^{-1} \right\| \| f(0) \|_{L^2(\Omega)}$$

$$- \left( \frac{1}{2} ((\delta_{\tau}(e^{-z\tau}))^\alpha + \mathcal{L})^{-1} \right)^k \left( ((\delta_{\tau}(e^{-z\tau}))^\alpha + \mathcal{L})^{-1} (\delta_{\tau}(e^{-z\tau}))^{-1} \right) dz \right\| \| f(0) \|_{L^2(\Omega)}$$

$$\leq I_{k,1} + I_{k,2} + I_{k,3}.$$

Lemma 2.1 and simple calculations imply

$$I_{k,1} \leq C \tau \int_{f_{\theta,k}^{-1}} \left| e^{\tau_n} \right| \left\| \left( \frac{1}{2} (z^\alpha + \mathcal{L})^{-1} \right)^k \right\| \left\| (z^\alpha + \mathcal{L})^{-1} \right\| \| dz \| \| f(0) \|_{L^2(\Omega)}$$

$$\leq C \tau \int_{f_{\theta,k}^{-1}} \left| e^{\tau_n} \right| \left| z \right|^{-(k+1)\alpha} \| dz \| \| f(0) \|_{L^2(\Omega)}$$

$$\leq C \tau \tau_n^{\alpha-1} \| f(0) \|_{L^2(\Omega)}.$$

According to the fact $|\frac{1}{z} - e^{-z\tau}| \leq C|z|$, one has

$$I_{k,2} \leq C \tau \tau_n^{\alpha-1} \| f(0) \|_{L^2(\Omega)}.$$

Using the fact $|z - \delta_{\tau}(e^{-z\tau})| \leq C|z|^2 \tau$ (see, e.g., Jin et al., 2016, 2017; Lubich et al., 1996) and doing simple calculations lead to

$$\left\| \left( \frac{1}{2} (z^\alpha + \mathcal{L})^{-1} \right)^k (z^\alpha + \mathcal{L})^{-1} z^{-1} \right\| \leq C \tau \tau_n^{\alpha-1} \| f(0) \|_{L^2(\Omega)}.$$

which yields

$$I_{k,3} \leq C \tau \tau_n^{\alpha-1} \| f(0) \|_{L^2(\Omega)}.$$

Similarly, one has

$$HI_k \leq C \tau \tau_n^{-1} \| G_0 \|_{L^2(\Omega)}.$$
As for $I_k$, we split it into two parts, i.e.,

$$I_k \leq C \left\| \int_0^t \left( \int_{\mathbb{R}^n} e^{\tau(n-t)} \left( \frac{1}{2} (\delta_\tau e^{-\tau})^\alpha + \mathcal{L}^{-1} \right)^k (\delta_\tau e^{-\tau})^\alpha + \mathcal{L}^{-1} \right) dz \right\|_{L^2(\Omega)}$$

$$\leq C \left\| \int_0^t \int_{\mathbb{R}^n} e^{\tau(n-t)} \left( \frac{1}{2} (\delta_\tau e^{-\tau})^\alpha + \mathcal{L}^{-1} \right)^k (\delta_\tau e^{-\tau})^\alpha + \mathcal{L}^{-1} \right) dz f'(s) ds \right\|_{L^2(\Omega)}$$

$$\leq C \left\| \int_0^t \int_{\mathbb{R}^n} e^{\tau(n-t)} \left( \frac{1}{2} (\delta_\tau e^{-\tau})^\alpha + \mathcal{L}^{-1} \right)^k (\delta_\tau e^{-\tau})^\alpha + \mathcal{L}^{-1} \right) dz f'(s) ds \right\|_{L^2(\Omega)}$$

$$\leq C \left\| \int_0^t \int_{\mathbb{R}^n} e^{\tau(n-t)} \left( \frac{1}{2} (\delta_\tau e^{-\tau})^\alpha + \mathcal{L}^{-1} \right)^k (\delta_\tau e^{-\tau})^\alpha + \mathcal{L}^{-1} \right) dz f'(s) ds \right\|_{L^2(\Omega)}$$

$$\leq C \left\| \int_0^t \int_{\mathbb{R}^n} e^{\tau(n-t)} \left( \frac{1}{2} (\delta_\tau e^{-\tau})^\alpha + \mathcal{L}^{-1} \right)^k (\delta_\tau e^{-\tau})^\alpha + \mathcal{L}^{-1} \right) dz f'(s) ds \right\|_{L^2(\Omega)}$$

$$\leq C \tau \int_0^t (t_n - s)^{\alpha - 1} \| f'(s) \|_{L^2(\Omega)} ds.$$

As for $I_{k, 2}$, the following fact

$$\tau \sum_{n=1}^\infty R(t_n) e^{-\tau_n} = \tau \sum_{n=1}^\infty \int_0^{t_n} f'(r) dr e^{-\tau_n}$$

$$= \tau \sum_{n=1}^\infty \int_{t_{j-1}}^{t_j} f'(r) dr e^{-\tau_n}$$

yields

$$I_{k, 2} \leq C \left\| \int_0^t \int_{\mathbb{R}^n} e^{\tau(n-t)} \left( \frac{1}{2} (\delta_\tau e^{-\tau})^\alpha + \mathcal{L}^{-1} \right)^k (\delta_\tau e^{-\tau})^\alpha + \mathcal{L}^{-1} \right) dz f'(s) ds \right\|_{L^2(\Omega)}$$

$$\leq C \tau \int_0^t (t_n - s)^{\alpha - 1} \| f'(s) \|_{L^2(\Omega)} ds.$$

As for $IV$, we introduce $e_t = G(t_k) - G^k$ and define $B_j$ by

$$B_j = \tau \int_{\mathbb{R}^n} e^{\tau_j} \left( \frac{1}{2} (\delta_\tau e^{-\tau})^\alpha + \mathcal{L}^{-1} \right)^{m+1} dz.$$  

Here we choose $m = \left\lfloor \frac{1}{\alpha} \right\rfloor$. It is easy to verify

$$\| B_j \| \leq C \tau \left( \frac{1}{\alpha} \right)^{m+1}.$$  

(3.6)
Thus, we can rewrite IV as

\[
IV \leq C \sum_{j=1}^{n} \left\| \int_{t_{j-1}}^{t_j} \int_{I_{0,x}} e^{i(t_0-s)} \left( \frac{1}{2} (Z^\alpha + L^\alpha)^{-1} \right)^{m+1} d\tau G(s) ds - B_{n-j} G^j \right\|_{L^2(\Omega)}
\]

\[
\leq C \sum_{j=1}^{n} \left\| \int_{t_{j-1}}^{t_j} \int_{I_{0,x}} e^{i(t_0-s)} \left( \frac{1}{2} (Z^\alpha + L^\alpha)^{-1} \right)^{m+1} d\tau (G(s) - G(t_j)) ds \right\|_{L^2(\Omega)}
\]

\[
+ C \sum_{j=1}^{n} \left\| \left( \int_{t_{j-1}}^{t_j} \int_{I_{0,x}} e^{i(t_0-s)} \left( \frac{1}{2} (Z^\alpha + L^\alpha)^{-1} \right)^{m+1} d\tau ds - B_{n-j} \right) G(t_j) \right\|_{L^2(\Omega)}
\]

\[
+ C \sum_{j=1}^{n} \left\| B_{n-j} \right\|_{L^2(\Omega)}
\]

\[
\leq IV_1 + IV_2 + IV_3.
\]

Using Theorem 2.2, one can get

\[
IV_1 \leq C \left\| \int_{t_0}^{t_1} \int_{I_{0,x}} e^{i(t_0-s)} \left( \frac{1}{2} (Z^\alpha + L^\alpha)^{-1} \right)^{m+1} d\tau (G(s) - G(t_1)) ds \right\|_{L^2(\Omega)}
\]

\[
+ \sum_{j=2}^{n} C \left\| \int_{t_{j-1}}^{t_j} \int_{I_{0,x}} e^{i(t_0-s)} \left( \frac{1}{2} (Z^\alpha + L^\alpha)^{-1} \right)^{m+1} d\tau (G(s) - G(t_j)) ds \right\|_{L^2(\Omega)}
\]

\[
\leq C \int_{t_0}^{t_1} \int_{I_{0,x}} |e^{i(t_0-s)}||s|^{-\alpha}\left( 1 + \frac{1}{2} (s^\alpha + \tau^\alpha)^{-1} \right)^{m+1} d\tau (G(s) + \|G(s)\|_{L^2(\Omega)} + \|G(t_1)\|_{L^2(\Omega)}) ds
\]

\[
+ \sum_{j=2}^{n} C \int_{t_{j-1}}^{t_j} \int_{I_{0,x}} |e^{i(t_0-s)}||s|^{-\alpha}\left( 1 + \frac{1}{2} (s^\alpha + \tau^\alpha)^{-1} \right)^{m+1} d\tau (G'(r) + \|G'(r)\|_{L^2(\Omega)}) dr ds
\]

\[
\leq C \frac{\tau}{(1+\alpha)\tau} \left( \|G(s)\|_{L^2(\Omega)} + \|G(t_1)\|_{L^2(\Omega)}) + \sum_{j=2}^{n} C \int_{t_{j-1}}^{t_j} \int_{I_{0,x}} |e^{i(t_0-s)}||s|^{-\alpha}\left( 1 + \frac{1}{2} (s^\alpha + \tau^\alpha)^{-1} \right)^{m+1} d\tau (G'(r) + \|G'(r)\|_{L^2(\Omega)}) dr ds
\]

\[
\leq C \tau \left( \ln(n) \|G_0\|_{L^2(\Omega)} + \|f(0)\|_{L^2(\Omega)} + \int_{0}^{t_0} \|f'(s)\|_{L^2(\Omega)} ds \right).
\]
Simple calculations lead to

\[ IV_2 \]
\[
\leq C \sum_{j=1}^{n} \left| \int_{t_{j-1}}^{t_j} \int_{\Gamma_{k,x}} e^{z(t_n-s)} \left( \frac{1}{2} (\varepsilon^{\alpha} + \mathcal{L}^{-1}) \right)^{m+1} dz \right| \left| G(t_j) \right|_{L^2(\Omega)} \\
- \tau \int_{t_{j-1}}^{t_j} e^{z(t_n-t_j)} \left( \frac{1}{2} (\varepsilon^{\alpha} + \mathcal{L}^{-1}) \right)^{m+1} dz \left| G(t_j) \right|_{L^2(\Omega)} \\
\leq C \sum_{j=1}^{n} \left| \int_{t_{j-1}}^{t_j} \int_{\Gamma_{k,x}} e^{z(t_n-s)} \left( \frac{1}{2} (\varepsilon^{\alpha} + \mathcal{L}^{-1}) \right)^{m+1} dz \right| \left| G(t_j) \right|_{L^2(\Omega)} \\
+ C \sum_{j=1}^{n} \left| \int_{t_{j-1}}^{t_j} \int_{\Gamma_{k,x}} e^{z(t_n-s)} - e^{z(t_n-t_j)} \left( \frac{1}{2} (\varepsilon^{\alpha} + \mathcal{L}^{-1}) \right)^{m+1} dz \right| \left| G(t_j) \right|_{L^2(\Omega)} \\
+ C \sum_{j=1}^{n} \left| \int_{t_{j-1}}^{t_j} \int_{\Gamma_{k,x}} e^{z(t_n-s)} \left( \frac{1}{2} (\varepsilon^{\alpha} + \mathcal{L}^{-1}) \right)^{m+1} dz \right| \left| G(t_j) \right|_{L^2(\Omega)} \\
\leq C^2 \sum_{j=1}^{n} \left( t_n - t_j + \tau \right)^{(m+1)\alpha-2} \left| G(t_j) \right|_{L^2(\Omega)} + C \tau \sum_{j=1}^{n} \int_{t_{j-1}}^{t_j} \left( t_n - s \right)^{(m+1)\alpha-2} ds \left| G(t_j) \right|_{L^2(\Omega)} \\
\leq C \tau \left( \left| G_0 \right|_{L^2(\Omega)} + \left| f(0) \right|_{L^2(\Omega)} + \int_{0}^{t_n} \left| f'(s) \right|_{L^2(\Omega)} ds \right) .
\]

As for \( IV_3 \), using (3.6), one has

\[ IV_3 \leq C \tau \sum_{j=1}^{n} \left( t_n - t_j \right)^{(m+1)\alpha-1} \left| e_j \right|_{L^2(\Omega)} .
\]

Thus combining the discrete Grönwall’s inequality (see, e.g., Thomée, 2006), the desired result is reached. \( \square \)

4. Fully-discrete scheme and error analysis

In this section, we provide the fully-discrete scheme by using local discontinuous Galerkin (LDG) method to discretize the operator \( \mathcal{L} \) and discuss the resulting error estimates.

Introduce a well approximation of the physical domain \( \Omega \) by the computational domain \( \Omega_h \) and the rectangle meshes are used. Let mesh size \( h = 1/N \) \( (N \in \mathbb{N}^+) \), \( x_i = v_i = ih \), \( (i = 0, 1, \ldots, N) \) and the elements

\[ I_{i,j} = (x_{i-1}, x_i) \times (v_{j-1}, v_j) \quad i, j = 1, 2, \ldots, N .\]

The polynomial space \( \mathbb{P}_k(I_{i,j}) \) consists of polynomials in \( I_{i,j} \) of degree at most \( k \) \( (k \geq 1) \) and the discontinuous finite element space \( V_{h,k} \) can be defined by

\[ V_{h,k} = \{ v : \Omega_h \rightarrow \mathbb{R} | v|_{I_{i,j}} \in \mathbb{P}_k(I_{i,j}), i, j = 1, \ldots, N \} .\]
Let $\mathbf{P}^n = \{P^n_x, P^n_i\} = \nabla G^n$. According to (3.1) and the definition of $L^v$, we have

$$
\begin{cases}
\left( \sum_{k=0}^{n-1} d_k^{(x)} (G^{n-k} - G^0), \mu \right)_{L_i^j} + (v P^n_x, \mu)_{L_i^j} - (v P^n_x, \mu)_{h_i^j} \\
+ \left( P^n_v \frac{\partial}{\partial v} \mu \right)_{L_i^j} - \int_{x_{i-1}}^{x_i} P^n_v \mu \left|_{v=v_{j-1}} \right. d x = (f^n, \mu)_{h_i^j} + (G^n, \mu)_{h_i^j} \quad (4.1)
\end{cases}
$$

for all $\mu \in H^1(\Omega)$ and $v \in (H^1(\Omega))^2$. Here $\mathbf{n}$ means the outward unit vector of $\partial L_i^j$. Let $\{G^n_h, P^n_h\} = \{G^n_h, \{P^n_{x,h}, P^n_{v,h}\}\}$ be the approximation of $\{G^n, P^n\}$. Then we can write the LDG scheme as: Find $\{G^n_h, P^n_h\} \in V_{h,k} \times (V_{h,k})^2$ such that

$$
\begin{cases}
\left( \sum_{k=0}^{n-1} d_k^{(x)} (G^{n-k}_h - G^0_h), \mu_h \right)_{L_i^j} + (v P^n_{x,h}, \mu_h)_{L_i^j} - (v P^n_{x,h}, \mu_h)_{h_i^j} \\
- \left( \frac{\partial}{\partial v} P^n_{v,h}, \mu_h \right)_{L_i^j} + \int_{x_{i-1}}^{x_i} (P^n_{v,h} - \tilde{P}^n_{v,h}) \mu_h \left|_{v=v_{j-1}} \right. d x = (f^n, \mu_h)_{h_i^j} + (G^n_h, \mu_h)_{h_i^j} \quad (4.2)
\end{cases}
$$

for all $\mu_h \in V_{h,k}$ and $v_h \in (V_{h,k})^2$. Here we choose the fluxes (see, e.g., Castillo et al., 2001; Cockburn & Shu, 1998)

$$
\begin{align*}
G^n_h(x_i, v) &= G^n_h(x_i^-, v) = \lim_{x \to x_i^-} G^n_h(x, v) \quad i = 1, \ldots, N, \\
G^n_h(x_0, v) &= G^n_h(x_0, v),
\end{align*}
$$

and

$$
\begin{align*}
\hat{G}^n_h(x, v_j) &= \hat{G}^n_h(x, v_j^-) = \lim_{v \to v_j^-} G^n_h(x, v) \quad j = 1, \ldots, N - 1, \\
\hat{G}^n_h(x, v_N) &= \hat{G}^n_h(x, v_N) = 0, \\
\hat{P}^n_{v,h}(x, v_j) &= P^n_{v,h}(x, v_j^-) = \lim_{v \to v_j^-} P^n_{v,h}(x, v) \quad j = 1, \ldots, N, \\
\hat{P}^n_{v,h}(x, v_0) &= P^n_{v,h}(x, v_0^-) + \frac{\hat{\partial} G^n_h(x, v_0^-)}{h},
\end{align*}
$$

where $\Theta$ is a positive constant.
Denote $\phi_h = \{G^n_h, P^n_h\}_{k=1}^m$ and $\psi_h = \{\mu_h, v_h, \eta_h\}$. Introduce

$$B_n(\phi_h, \psi_h) = \sum_{i,j=1}^{N} \left( \sum_{k=0}^{n-1} d_k^{(\alpha)}(G^0_h - G^0_h, \mu_h)_{i,j} + (vP^n_{y,h}; \mu_h)_{i,j} - (vP^n_{y,h}; \mu_h)_{i,j} ight)$$

Then we have

Using Cauchy’s integral theorem and doing simple calculations lead to

Assume that

Proof. Assume that $v^n$ satisfies

Thus we can rewrite (4.2) as

To prove stability of the scheme, we first provide a new discrete Grönwall’s inequality.

**Lemma 4.1** Let $u^n \geq 0$ ($n = 0, 1, \ldots$) satisfy

Then we have

$$u^n \leq C u^0.$$  

**Proof.** Assume that $v^n$ satisfies

Multiplying $\xi^n$ on both sides of (4.6) and summing $n$ from 1 to $\infty$, we obtain

Combining the definition of $d_k^{(\alpha)}$, i.e., (3.2), one can get

Using Cauchy’s integral theorem and doing simple calculations lead to

$$v^n = \frac{1}{2\pi i} \int_{R_y} e^{\delta z} (\delta z (e^{-\delta z}))^{-1} u^0 dz + \frac{\tau}{2\pi i} \int_{R_y} e^{\delta z} (\delta z (e^{-\delta z}))^{-1} u^0 e^{-\delta z} dz.$$
Thus by using $C_1|z| \leq |\delta_t(e^{-\tau z})| \leq C_2|z|$ with $C_1, C_2$ being two positive constants for $z \in \Gamma_{\theta,k}^+$ (see, e.g., Jin et al., 2016, 2017) and simple calculations, there holds

$$|v^n| \leq C|u^0| + C\tau \sum_{i=0}^{n-1} |u^{n-i}|.$$

Subtracting (4.6) from (4.5), we have

$$\sum_{k=0}^{n-1} d_k^{(\alpha)} (u^{n-k} - v^{n-k}) \leq 0.$$

Further, Lemma 3.1 gives

$$u^n \leq v^n \leq C|u^0| + C\tau \sum_{i=0}^{n-1} |u^{n-i}|.$$

Combining the discrete Grönewall inequality (see, e.g., Thomée, 2006), we have

$$u^n \leq C|u^0|.$$

This completes the proof.

Thanks to above Lemma 4.1, we can get the following stability result.

**Theorem 4.1** The scheme (4.2) with fluxes (4.3) and (4.4) is $L^2$ stable, i.e.,

$$\|e^n_G\|_{L^2(\Omega)} \leq C\|e^0_G\|_{L^2(\Omega)},$$

where $e^n_G = G^n_h - \tilde{G}^n_h$.

**Proof.** Choosing $\mu = e^n_G, \nu = \{\nu e^n_G - \nu e^n_V\}$, and $\eta = e^n_P$, one has

$$\mathcal{B}_n(\mu, \nu) = \sum_{i,j=1}^{N} \left( \left( \sum_{k=0}^{n-1} d_k^{(\alpha)} (e^n_G - e^n_V), e^n_G \right)_{h,i,j} + (\nu e^n_G, e^n_V)_{h,i,j} - (\nu e^n_V, e^n_G)_{h,i,j} + \frac{i}{\tau} \int_{t_{i-1}}^{t_i} (e^n_G - \tilde{e}^n_G) (e^n_V - \tilde{e}^n_V) |v|_{\Gamma_{i,j}} dx \right) = 0.$$

By the fluxes (4.3) and (4.4), we have

$$\sum_{i,j=1}^{N} \left( - \left( \frac{\partial}{\partial v} e^n_G, e^n_G \right)_{h,i,j} + \frac{i}{\tau} \int_{t_{i-1}}^{t_i} (e^n_G - \tilde{e}^n_G) (e^n_V - \tilde{e}^n_V) |v|_{\Gamma_{i,j}} dx \right) = \sum_{i=1}^{N} \int_{t_{i-1}}^{t_i} \frac{\partial (e^n_P (v^n) )^2}{h} dx.$$
and
\[
\sum_{i,j=1}^{N} \left( (\nabla \epsilon_G^n, \nu_h)_{l_{ij}} - (\epsilon_G^n - \hat{\epsilon}_G^n, \nu_h)_{\partial l_{ij}} \right) \\
= \frac{1}{2} \sum_{j=1}^{N} \int_{v_j}^{
u_j} \left( \sum_{i=1}^{N-1} \nu_j(\hat{\epsilon}_G^n(x_j^-) - \epsilon_G^n(x_j)) \right)^2 + \nu_j(\epsilon_G^n(x_j^-) - \epsilon_G^n(x_j))^2 \, dv \\
\quad + \frac{1}{2} \sum_{i=1}^{N} \int_{x_i}^{x_i+1} \left( \sum_{j=1}^{N-1} \nu_j(\hat{\epsilon}_G^n(v_j^-) - \epsilon_G^n(v_j)) \right)^2 + \nu_j(\epsilon_G^n(v_j^-) - \epsilon_G^n(v_j))^2 \, dx \\
\quad + \frac{1}{2} \sum_{i,j=1}^{N} (\hat{\epsilon}_G^n, \epsilon_G^n)_{l_{ij}}.
\]

Thus
\[
\sum_{i,j=1}^{N} \left( d_{ij}^{(\alpha)} \epsilon_G^n, \epsilon_G^n \right)_{l_{ij}} \\
\leq \sum_{i,j=1}^{N} \left( \sum_{k=0}^{n-1} d_k^{(\alpha)} \epsilon_G^n, \epsilon_G^n \right)_{l_{ij}} \\
\leq \sum_{k=0}^{n-1} \left( \sum_{i,j=1}^{N} d_k^{(\alpha)} \left( \| \epsilon_G^n \|_{L^2(l_{ij})}^2 \right) - \sum_{i,j=1}^{N} \left( \| \epsilon_G^n \|_{L^2(l_{ij})}^2 \right) \right) \\
\leq \frac{1}{2} \sum_{k=0}^{n-1} \left( \sum_{i,j=1}^{N} d_k^{(\alpha)} \left( \| \epsilon_G^{n-k} \|_{L^2(l_{ij})}^2 \right) - \sum_{i,j=1}^{N} \left( \| \epsilon_G^n \|_{L^2(l_{ij})}^2 \right) \right),
\]

which leads to
\[
\sum_{k=0}^{n-1} \sum_{i,j=1}^{N} d_k^{(\alpha)} \left( \| \epsilon_G^{n-k} \|_{L^2(l_{ij})}^2 \right) \leq \sum_{i,j=1}^{N} \left( \| \epsilon_G^n \|_{L^2(l_{ij})}^2 \right).
\]

Further combining Lemma 4.1, we can obtain the desired result. \qed

At last, we provide the error estimate for the fully-discrete scheme (4.2). Introduce $L^2$ projection operator $\mathcal{P}_x$ in one dimension as, for all $(x_{i-1}, x_i) \in (0, 1)$
\[
\int_{x_{i-1}}^{x_i} (\mathcal{P}_x \mu - \mu) \, dx = 0 \quad \forall \nu \in \mathbb{P}_k(x_{i-1}, x_i).
\]

Define the projection operators $\mathcal{P}_x^+$ and $\mathcal{P}_x^-$ as
\[
\int_{x_{i-1}}^{x_i} (\mathcal{P}_x^+ \mu - \mu) \, dx = 0 \quad \forall \nu \in \mathbb{P}_{k-1}(x_{i-1}, x_i) \quad \text{and} \quad \mathcal{P}_x^+ \mu(x_{i-1}) = \mu(x_{i-1}),
\]

and
\[
\int_{x_{i-1}}^{x_i} (\mathcal{P}_x^- \mu - \mu) \, dx = 0 \quad \forall \nu \in \mathbb{P}_{k-1}(x_{i-1}, x_i) \quad \text{and} \quad \mathcal{P}_x^- \mu(x_i) = \mu(x_i).
\]

Moreover, define the following projections in two dimensions by tensor products
\[
\Pi = \mathcal{P}_x \otimes \mathcal{P}_v^+ , \quad \Pi_0 = \mathcal{P}_x \otimes \mathcal{P}_v, \quad \Pi_0^- = \mathcal{P}_x \otimes \mathcal{P}_v^-.
\]
LEMMA 4.2 (see, e.g., Cockburn et al., 2001) For any \( u \in \mathbb{P}_{k+1}(I_{i,j}) \) and \( \nu = \{ \nu_x, \nu_y \} \in (\mathbb{P}_k(I_{i,j}))^2 \), we have

\[
\begin{align*}
\left( u - \Pi u, \frac{\partial}{\partial x} \nu_x \right)_{I_{i,j}} - \int_{\nu_{i,j}}^{\nu_{i,j+1}} (u - \Pi u) \nu_x \bigg|_{x_{i,j-1}}^{x_{i,j}} \, dv = 0, \\
\left( u - \Pi u, \frac{\partial}{\partial y} \nu_y \right)_{I_{i,j}} - \int_{\nu_{i,j}}^{\nu_{i,j+1}} (u - \Pi u) \nu_y \bigg|_{x_{i,j-1}}^{x_{i,j}} \, dx = 0,
\end{align*}
\]

and

\[
(u - \Pi u, \nabla \cdot \nu)_{I_{i,j}} - (u - \Pi u, n \cdot \nu)_{\partial I_{i,j}} = 0.
\]

THEOREM 4.2 Let \( G^n \) and \( G^n_h \) be the solutions of (3.1) and (4.2), respectively. If \( G^i \in H^{k+2}(\Omega) \) and \( P^i \in (H^{k+1}(\Omega))^2 \) for \( i = 0, 1, 2, \ldots, n \), then we have

\[
\| G^n - G^n_h \|_{L^2(\Omega)} \leq C h^{k+1}.
\]

**Proof.** Introduce

\[
e = \{ e^k_G, e^k_P \}_{k=1}^\infty = \{ G^k - G^k_h, P^k - P^k_h \}_{k=1}^\infty.
\]

From (4.1) and (4.2), it's easy to verify

\[
\mathcal{B}_n(e, \psi_h) = 0
\]

for \( \psi_h \in V_{h,k} \times (V_{h,k})^2 \). Taking \( \psi_h = \{ u_h, \nu_h \} = \{ \Pi e^k_G, \nu \Pi e^k_G, -\nu \Pi e^k_G, \Pi^*_e e^k_P \} \) and denoting \( \Pi e = \{ \Pi e^k_G, \{ \Pi e^k_P, \Pi^*_e e^k_P \} \}_{k=1}^\infty \), one can obtain

\[
\begin{align*}
\mathcal{B}_n(\Pi e, \psi_h) &= \mathcal{B}_n(e, \psi_h) + \mathcal{B}_n(\rho, \psi_h) \\
&= \mathcal{B}_n(\rho, \psi_h),
\end{align*}
\]

where

\[
\rho = \{ \rho^k_G, \rho^k_P \}_{k=1}^\infty = \{ \rho^k_G, \{ \rho^k_P, \rho^k_P \} \}_{k=1}^\infty = \{ \Pi G^k - G^k, \{ \Pi P^k - P^k, \Pi^*_e P^k - P^k \} \}_{k=1}^\infty.
\]

Similar to the derivations of Theorem 4.1, we have

\[
2 \mathcal{B}_n(\Pi e, \psi_h)
\]

\[
\geq \sum_{k=0}^{n-1} d_k^{(\alpha)} \left( \sum_{i,j=1}^N \| \Pi e_{i,j}^{n-k} \|_{L^2(I_{i,j})}^2 - \sum_{i,j=1}^N \| \Pi e_{i,j}^0 \|_{L^2(I_{i,j})}^2 + \sum_{i,j=1}^N \| \Pi e_{i,j}^n \|_{L^2(I_{i,j})}^2 \right)

+ \sum_{j=1}^{\nu_{i,j}} \int_{\nu_{i,j}}^{\nu_{i,j+1}} \left( \sum_{i=1}^{\nu_j} \left( \int_{x_{i-1}}^{x_i} \left( \Pi e_{G}(x_i^-) - \Pi e_{G}(x_i^+) \right)^2 + v \left( \Pi e_{G}(x_i^+) \right)^2 \right) \, dx \right) \, dv

+ \sum_{j=1}^{\nu_{i,j}} \int_{\nu_{i,j}}^{\nu_{i,j+1}} \left( \int_{x_{i-1}}^{x_i} \left( \Pi e_{G}(v_j^-) - \Pi e_{G}(v_j^+) \right)^2 + v \left( \Pi e_{G}(v_j^+) \right)^2 \right) \, dx

+ 2 \sum_{i,j=1}^N \| \Pi^*_e e^k_P \|_{L^2(I_{i,j})}^2.
\]
Furthermore, there holds

\[ \tau^\alpha \mathcal{B}_n(\rho, \psi_h) = \tau^\alpha \sum_{i,j=1}^N \left( \sum_{k=0}^{n-1} d_k^{(\alpha)} \left( (\rho^{n-k}_G - \rho^0_G), \mu_h \right)_{L_j} + (\nu \rho^n_F, \mu_h)_{L_j} - (\nu \rho^n_F, \mu_h)_{L_j} \right) \]

\[ - \left( \frac{\partial}{\partial \nu} \mu^n_{L_j}, \mu_h \right)_{L_j} + \int_{\Omega_{\eta}} (\rho^n_{L_j} - \hat{\rho}_G^n) \eta_h \big|_{\nu=v_{ij-1}} dx - (\rho^n_G, \mu_h)_{L_j} \]

\[ - (\rho^n_{L_j}, \eta_h)_{L_j} + \left( \frac{\partial}{\partial \nu} \rho^n_{L_j}, \eta_h \right)_{L_j} - \int_{\Omega_{\eta}} (\rho^n_G - \hat{\rho}_G^n) \eta_h \big|_{\nu=v_{ij-1}} dx \]

\[ \leq I + II + III + IV + V + VI + VII, \]

where

\[ I = \tau^\alpha \sum_{i,j=1}^N \left( (\nu \rho^n_F, \mu_h)_{L_j} - (\nu \rho^n_F, \mu_h)_{L_j} - (\nu \rho^n_F, \psi_h)_{L_j} - (\nu \rho^n_F, \mu_h)_{L_j} \right), \]

\[ II = \tau^\alpha \sum_{i,j=1}^N \left( - \int_{\Omega_{\eta}} \rho^n_{L_j} \mu_h \big|_{\nu=v_{ij-1}} dx \right), \]

\[ III = - \tau^\alpha \sum_{i,j=1}^N \left( (\rho^n_G, \nabla \cdot \psi_h)_{L_j} - (\rho^n_G, \nabla \cdot \psi_h)_{L_j} \right), \]

\[ IV = - \tau^\alpha \sum_{i,j=1}^N \left( \left( \rho^n_G, \frac{\partial}{\partial \nu} \eta_h \right)_{L_j} - \int_{\Omega_{\eta}} \hat{\rho}_G^n \eta_h \big|_{\nu=v_{ij-1}} dx \right), \]

\[ V = \tau^\alpha \sum_{i,j=1}^N \left( \left( \rho^n_G, \frac{\partial}{\partial \nu} \mu_h \right)_{L_j} \right), \]

\[ VI = \tau^\alpha \sum_{i,j=1}^N \left( - (\rho^n_{L_j}, \eta_h)_{L_j} \right), \]

\[ VII = \tau^\alpha \sum_{i,j=1}^N \sum_{k=0}^{n-1} d_k^{(\alpha)} \left( (\rho^{n-k}_G - \rho^0_G), \mu_h \right)_{L_j} \cdot \]

The property of the projection (see, e.g., Dong & Shu, 2009), the Cauchy-Schwarz inequality, and the Young inequality show that for \( \epsilon > 0 \),

\[ I \leq C \epsilon^{-1} \tau^\alpha h^{2k+2} + \epsilon \tau^\alpha \| \Pi e^\alpha \|_{L^2(\Omega)}^2. \]

According to (4.4), for \( \epsilon > 0 \), there exists

\[ II \leq C \epsilon^{-1} \tau^\alpha h^{2k+2} + \tau^\alpha \epsilon \sum_{i=1}^N \int_{\Omega_{\eta}} \left( \frac{2 \partial}{\partial h} \right) (\Pi e^\alpha (v^0_0))^2 dx. \]
According to Lemma 4.2, for $\varepsilon > 0$, one has

$$
III \leq C \tau^\alpha \sum_{i,j=1}^N \left| (\rho^n_{G, \nabla \cdot \mathbf{v}_h, \rho^n G, \mathbf{n} \cdot \mathbf{v}_h)_{\partial \Omega_{i,j}} - (\tilde{\rho}^n_{G, \nabla \cdot \mathbf{v}_h, \rho^n G, \mathbf{n} \cdot \mathbf{v}_h)_{\partial \Omega_{i,j}} \right|
$$

$$
\leq C \tau^\alpha \sum_{i,j=1}^N \left| (\nabla \cdot \rho^n_{G, \nabla \cdot \mathbf{v}_h, \rho^n G, \mathbf{n} \cdot \mathbf{v}_h)_{\partial \Omega_{i,j}} - (\nabla \cdot \tilde{\rho}^n_{G, \nabla \cdot \mathbf{v}_h, \rho^n G, \mathbf{n} \cdot \mathbf{v}_h)_{\partial \Omega_{i,j}} \right|
$$

$$
+ C \tau^\alpha \sum_{i,j=1}^N \left| (\rho^n_{G, \Pi e^n G})_{\Omega_{i,j}} \right|
$$

$$
\leq C \varepsilon^a \alpha h^{2k+2} + \tau^\alpha \varepsilon \|\Pi e^n G\|_{L^2(\Omega)}^2.
$$

Similarly, for $\varepsilon > 0$, there holds

$$
IV \leq C \varepsilon^{-1} \alpha h^{2k+2} + \tau^\alpha \varepsilon \|\Pi e^n G\|_{L^2(\Omega)}^2.
$$

The property of projection (see, e.g., Dong & Shu, 2009) implies

$$
V = 0.
$$

As for $VI$, the Cauchy-Schwarz inequality, the Young inequality, and the property of projection lead to that for $\varepsilon > 0$,

$$
VI \leq C \varepsilon^{-1} \alpha h^{2k+2} + \tau^\alpha \varepsilon \|\Pi e^n G\|_{L^2(\Omega)}^2.
$$

Using the definition of $d^{(a)}_k$ and Lemma 3.1, we have, for $\varepsilon > 0$,

$$
VII \leq C \varepsilon^{-1} h^{2k+2} + \varepsilon \|\Pi e^n G\|_{L^2(\Omega)}^2.
$$

Combining (4.7) and choosing $\varepsilon > 0$ small enough, we can obtain

$$
\tau^\alpha \sum_{k=0}^{n-1} d^{(a)}_k \left( \sum_{i,j=1}^N \|\Pi e^{0-k}_G\|_{L^2(\Omega)}^2 - \sum_{i,j=1}^N \|\Pi e^0_G\|_{L^2(\Omega)}^2 \right)
$$

$$
- \left( \frac{3}{2} \tau^\alpha + \varepsilon \right) \sum_{i,j=1}^N \|\Pi e^0_G\|_{L^2(\Omega)}^2 \leq Ch^{2k+2},
$$

which leads to

$$
\tau^\alpha \sum_{k=0}^{n-1} d^{(a)}_k \left( \sum_{i,j=1}^N \|\Pi e^{0-k}_G\|_{L^2(\Omega)}^2 - \sum_{i,j=1}^N \|\Pi e^0_G\|_{L^2(\Omega)}^2 \right)
$$

$$
- \left( \frac{3}{2} \tau^\alpha + \varepsilon \right) \sum_{i,j=1}^N \left( \|\Pi e^0_G\|_{L^2(\Omega)}^2 - \|\Pi e^0_G\|_{L^2(\Omega)}^2 \right) \leq Ch^{2k+2}.
$$

Further, the definition of $d^{(a)}_k$ yields

$$
\|\Pi e^{0-k}_G\|_{L^2(\Omega)}^2 \leq Ch^{2k+2}.
$$

Thus combining the above estimate and the property of projection leads to the desired result. \qed
5. Numerical Experiments

In this section, we provide two examples to verify the temporal and spatial convergence rates, respectively. In the following, we take $\vartheta = 1$.

EXAMPLE 5.1 Here we show temporal convergence rates for the system (1.1) with boundary condition (1.2). We take $T = 1$, $k = 1$, $h = 1/16$, and for the initial condition consider the following three cases, i.e.,

(a) $G_0 = x \times \sin(\pi v)$, $f = 0$;

(b) $G_0 = \chi_{(0.5,1)}(x)\chi_{(0.0,0.5)}(v)$, $f = 0$;

(c) $G_0 = 0$, $f = \chi_{(0.5,1)}(x)\chi_{(0.0,0.5)}(v)t^{0.8}$,

where $\chi_{(a,b)}$ is the characteristic function on $(a,b)$. Because the exact solution is unknown, the errors and convergence rates can be calculated by

$$E_\tau = \|G_\tau - G_{\tau/2}\|_{L^2(\Omega)}$$

and

$$\text{rate} = \frac{\ln(E_\tau/E_{\tau/2})}{\ln(2)}$$

where $G_\tau$ denotes the numerical solution of $G$ at time $T$ with step size $\tau$.

We first provide the numerical results for the system (1.1) with boundary condition (1.2) and initial condition (a). From the errors and convergence rates shown in Table 1, it can be noted that all the results agree with Theorem 3.1. Then we consider the system with the initial condition (b). Although the initial condition is nonsmooth, the convergence rates shown in Table 2 are still $O(\tau)$, which validate the results of Theorem 3.1. Next, for the initial condition (c), the corresponding convergence rates presented in Table 3 are same with the predicted ones in Theorem 3.1.

| $\alpha$ | 1/ $\tau$ | 10   | 20   | 40   | 80   | 160  |
|----------|-----------|------|------|------|------|------|
| 0.3      | 2.726E-04 | 1.329E-04 | 6.564E-05 | 3.262E-05 | 1.626E-05 |
| Rate     | 1.05360   | 1.0179 | 1.0089 | 1.0045 |
| 0.5      | 4.442E-04 | 2.138E-04 | 1.049E-04 | 5.197E-05 | 2.586E-05 |
| Rate     | 1.0550    | 1.0272 | 1.0135 | 1.0067 |
| 0.8      | 5.479E-04 | 2.487E-04 | 1.187E-04 | 5.803E-05 | 2.869E-05 |
| Rate     | 1.1395    | 1.0668 | 1.0326 | 1.0161 |

EXAMPLE 5.2 Here we validate the spatial convergence rates for the scheme (4.2). We take $T = 1$,

$$G_0 = \sin(\pi x)\sin(\pi v)$$
Table 2. Temporal errors and convergence rates for the system (1.1) with boundary condition (1.2) and initial condition (b)

| $\alpha \cdot 1/\tau$ | 10    | 20    | 40    | 80    | 160   |
|------------------------|-------|-------|-------|-------|-------|
| 0.2                    | 1.264E-04 | 6.192E-05 | 3.065E-05 | 1.525E-05 | 7.603E-06 |
| Rate                   | 1.0294 | 1.0147 | 1.0073 | 1.0037 |       |
| 0.4                    | 2.531E-04 | 1.227E-04 | 6.041E-05 | 2.997E-05 | 1.493E-05 |
| Rate                   | 1.0447 | 1.0222 | 1.0110 | 1.0055 |       |
| 0.6                    | 3.521E-04 | 1.677E-04 | 8.184E-05 | 4.044E-05 | 2.010E-05 |
| Rate                   | 1.0705 | 1.0346 | 1.0172 | 1.0085 |       |

Table 3. Temporal errors and convergence rates for the system (1.1) with boundary condition (1.2) and initial condition (c)

| $\alpha \cdot 1/\tau$ | 10    | 20    | 40    | 80    | 160   |
|------------------------|-------|-------|-------|-------|-------|
| 0.2                    | 6.500E-06 | 3.352E-06 | 1.705E-06 | 8.610E-07 | 4.329E-07 |
| Rate                   | 0.9556 | 0.9751 | 0.9858 | 0.9919 |       |
| 0.5                    | 9.831E-06 | 5.076E-06 | 2.584E-06 | 1.306E-06 | 6.567E-07 |
| Rate                   | 0.9537 | 0.9740 | 0.9850 | 0.9913 |       |
| 0.7                    | 6.149E-06 | 3.191E-06 | 1.630E-06 | 8.253E-07 | 4.158E-07 |
| Rate                   | 0.9463 | 0.9693 | 0.9818 | 0.9890 |       |

and

$$f = \Gamma(\alpha + 1) \sin(\pi x) \sin(\pi v)$$

$$+ \left( \pi^2 \sin(\pi x) \sin(\pi v) + \pi \cos(\pi x) \sin(\pi v) \right) + \left( -\pi \cos(\pi x) \sin(\pi v) - \sin(\pi x) \sin(\pi v) \right) t^{\alpha + 1},$$

which implies the exact solution

$$G = (t^\alpha + 1) \sin(\pi x) \sin(\pi v).$$

In Table 4, we choose the order of approximation polynomial $k = 1$ and $\tau = \frac{1}{100}$. We find the convergence rates are $O(h^2)$, which are same with the theoretical ones in Theorem 4.2. In Table 5, we take the order of approximation polynomial $k = 2$ and to investigate the convergence in space and eliminate the influence from temporal discretization, we take $\tau = \frac{1}{200}$. From Table 5, we see the convergence rates are $O(h^3)$, which are consistent with the predicted ones.

6. Conclusions

We provide the regularity estimates and numerical analyses for fractional Klein-Kramers equation. By introducing a new positive operator $L$ to overcome hypocoercivity of the original one and building its resolvent estimate, we give spatial and temporal regularity of the solution. Then, backward Euler convolution quadrature method and local discontinuous Galerkin method are used to approximate Riemann-
| $\alpha \cdot 1/h$ | 4     | 8     | 12    | 16    | 20    |
|------------------|-------|-------|-------|-------|-------|
| 0.3              | 1.032E-01 | 2.625E-02 | 1.175E-02 | 6.635E-03 | 4.259E-03 |
| Rate             | 1.9755 | 1.9830 | 1.9859 | 1.9867 |       |
| 0.5              | 1.032E-01 | 2.623E-02 | 1.174E-02 | 6.627E-03 | 4.252E-03 |
| Rate             | 1.9757 | 1.9835 | 1.9869 | 1.9884 |       |
| 0.7              | 1.031E-01 | 2.622E-02 | 1.173E-02 | 6.621E-03 | 4.247E-03 |
| Rate             | 1.9758 | 1.9839 | 1.9876 | 1.9896 |       |

| $\alpha \cdot 1/h$ | 4     | 8     | 12    | 16    | 20    |
|------------------|-------|-------|-------|-------|-------|
| 0.4              | 3.372E-03 | 4.285E-04 | 1.269E-04 | 5.365E-05 | 2.779E-05 |
| Rate             | 2.9763 | 3.0014 | 2.9927 | 2.9477 |       |
| 0.6              | 3.371E-03 | 4.281E-04 | 1.266E-04 | 5.331E-05 | 2.730E-05 |
| Rate             | 2.9770 | 3.0048 | 3.0069 | 2.9989 |       |
| 0.8              | 3.370E-03 | 4.280E-04 | 1.265E-04 | 5.321E-05 | 2.719E-05 |
| Rate             | 2.9772 | 3.0058 | 3.0101 | 3.0089 |       |

Liouville fractional derivative and the operator $\mathcal{L}$, respectively, and the complete error analyses are also built. Finally, we perform the numerical experiments, which support the theoretical results.

Acknowledgements

This work was supported by National Natural Science Foundation of China under Grant No. 12071195, AI and Big Data Funds under Grant No. 2019620005000775, and Fundamental Research Funds for the Central Universities under Grant Nos. Izujbky-2021-it26 and Izujbky-2021-kb15.

REFERENCES

CASTILLO, P., COCKBURN, B., SCHÖTZAU, D. & SCHWAB, C. (2001) Optimal a priori error estimates for the $hp$-version of the local discontinuous Galerkin method for convection–diffusion problems. *Math. Comp.*, 71, 455–479.

CHEN, S., LIU, F., ZHUANG, P. & ANH, V. (2009) Finite difference approximations for the fractional Fokker–Planck equation. *Appl. Math. Model.*, 33, 256–273.

COCKBURN, B., KANSCHAT, G., PERUGIA, I. & SCHÖTZAU, D. (2001) Superconvergence of the local discontinuous Galerkin method for elliptic problems on Cartesian grids. *SIAM J. Numer. Anal.*, 39, 264–285.

COCKBURN, B. & SHU, C.-W. (1998) The local discontinuous Galerkin method for time-dependent convection-diffusion systems. *SIAM J. Numer. Anal.*, 35, 2440–2463.

DENG, W., CHEN, M. & BARKAI, E. (2015) Numerical algorithms for the forward and backward fractional Feynman–Kac equations. *J. Sci. Comput.*, 62, 718–746.

DENG, W. & LI, C. (2011) Finite difference methods and their physical constraints for the fractional Klein-Kramers equation. *Numer. Methods Partial Differential Equations*, 27, 1561–1583.
DONG, B. & SHU, C.-W. (2009) Analysis of a local discontinuous Galerkin method for linear time-dependent fourth-order problems. *SIAM J. Numer. Anal.*, 47, 3240–3268.

ELLIOTT, C. M. & LARSSON, S. (1992) Error estimates with smooth and nonsmooth data for a finite element method for the Cahn-Hilliard equation. *Math. Comp.*, 58, 603–630.

GAO, G.-H. & SUN, Z.-Z. (2012) A finite difference approach for the initial-boundary value problem of the fractional Klein-Kramers equation in phase space. *Cent. Eur. J. Math.*, 10, 101–115.

JIN, B., LAZAROV, R. & ZHOU, Z. (2016) Two fully discrete schemes for fractional diffusion and diffusion-wave equations with nonsmooth data. *SIAM J. Sci. Comput.*, 38, A146–A170.

JIN, B., LI, B. & ZHOU, Z. (2017) Correction of high-order BDF convolution quadrature for fractional evolution equations. *SIAM J. Sci. Comput.*, 39, A3129–A3152.

Li, C., DENG, W. & Wu, Y. (2012) Finite difference approximations and dynamics simulations for the Lévy fractional Klein-Kramers equation. *Numer. Methods Partial Differential Equations*, 28, 1944–1965.

LUBICH, C. (1988a) Convolution quadrature and discretized operational calculus. I. *Numer. Math.*, 52, 129–145.

LUBICH, C. (1988b) Convolution quadrature and discretized operational calculus. II. *Numer. Math.*, 52, 413–425.

LUBICH, C., SLOAN, I. H. & THOMÉE, V. (1996) Nonsmooth data error estimates for approximations of an evolution equation with a positive-type memory term. *Math. Comp.*, 65, 1–18.

METZLER, R. & KLAFTER, J. (2000a) From a generalized Chapman–Kolmogorov equation to the fractional Klein–Kramers equation. *J. Phys. Chem. B*, 104, 3851–3857.

METZLER, R. & KLAFTER, J. (2000b) Subdiffusive transport close to thermal equilibrium: From the Langevin equation to fractional diffusion. *Phys. Rev. E*, 61, 6308–6311.

METZLER, R. & KLAFTER, J. (2000c) The random walk’s guide to anomalous diffusion: A fractional dynamics approach. *Phys. Rep.*, 339, 1–77.

NIKAN, O., TENREIRO MACHADO, J. A., GOLBABAI, A. & RASHIDINIA, J. (2021) Numerical evaluation of the fractional Klein–Kramers model arising in molecular dynamics. *J. Comput. Phys.*, 428, 109983.

PODLUBNY, I. (1999) *Fractional Differential Equations*. Mathematics in science and engineering series. San Diego and London: Academic.

THOMÉE, V. (2006) *Galerkin Finite Element Methods for Parabolic Problems*. Springer series in computational mathematics, 2nd edn. Berlin and Great Britain: Springer.