FRACTIONAL SENSITIVITY EQUATION METHOD: APPLICATIONS TO FRACTIONAL MODEL CONSTRUCTION

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Abstract. Fractional differential equations provide a tractable mathematical framework to describe anomalous behavior in complex physical systems, yet they introduce new sensitive model parameters, i.e. derivative orders, in addition to model coefficients. We formulate a sensitivity analysis of fractional models by developing a fractional sensitivity equation method. We obtain the adjoint fractional sensitivity equations, in which we present a fractional operator associated with logarithmic-power law kernel. We further construct a gradient-based optimization algorithm to compute an accurate parameter estimation in fractional model construction. We develop a fast, stable, and convergent Petrov-Galerkin spectral method to numerically solve the coupled system of original fractional model and its corresponding adjoint fractional sensitivity equations.

Key words. sensitive fractional orders, model error, logarithmic-power law kernel, Petrov-Galerkin spectral method, iterative algorithm, parameter estimation.

1. Introduction. The experimental observations in a divers number of complex physical systems reveal ubiquitous anomalous behavior in the associated underlying processes [62, 61], where the anomaly manifests itself in skewness and sharpness of heavy tailed distributions. Fractional differential equations, which generalize their integer order counterparts, construct a rigorous mathematical framework to formulate models that flawlessly describe such anomalies. The excellence of fractional operator in accurate prediction of non-locality and memory effects is the inherent non-local nature of singular power-law kernel, whose order is defined as fractional derivative order, i.e. fractional index. These operators are being extensively used in analysis and design of models for a wide range of multi-scale multi-physics phenomena. Examples include viscoelastic materials and wave propagation [39, 55, 41], non-Brownian transport phenomena in porous media and disordered materials [6, 41], non-Newtonian complex fluids with multi-phase applications and rheology [23, 52, 4, 17], multi-scale patterns in biological tissue [43, 44, 38, 4, 17], chaos/fractals and automatic control [31, 18]. However, the key challenges of such models are the excessive computational cost in numerically integrating the convolution operation, and more importantly, introducing fractional derivative orders as extra model parameters, whose values are essentially obtained from experimental data. The sensitivity assessment of fractional models with respect to fractional indecis can build a bridge between experiments and mathematical models to gear observable data via proper optimization techniques, and thus, systematically improve the existing models in both analysis and design approaches. We formulate a mathematical framework by developing a fractional sensitivity equation method, where we investigate the response sensitivity of fractional differential equations with respect to model parameters including derivative orders, and further construct an iterative algorithm in order to exploit the obtained sensitivity field in parameter estimation.

Fractional Sensitivity Analysis. Sensitivity assessment approaches are commonly categorized as, finite difference, continuum and discrete derivatives, and computational or automatic differentiation, where the sensitivity coefficients are generally defined as partial derivative of corresponding functions (model output) with respect to design/analysis parameters of inter-
Finite difference schemes use a first order Taylor series expansion to approximate the sensitivity coefficients, where accuracy depends strongly on step increment [40, 51]. Continuum and discrete derivative techniques however, differentiate the system response with respect to parameters, where the former, which is also known as sensitivity equation method (SEM, see [37, 72] and references therein), directly computes the derivatives and obtain a set of (coupled) adjoint continuum sensitivity equations; while the latter performs differentiation after discretization of original equation [53]. Automatic differentiation method also refers to a differentiation of the computer code [8, 10, 9]. Fig.2 in [56] provides a descriptive schematic of these different approaches. We extend the continuum derivative technique to develop a fractional sensitivity equation method (FSEM) in the context of fractional partial differential equations (FPDEs). To formulate the sensitivity analysis framework, we let q be a set of model parameters including fractional indices and obtain the adjoint fractional sensitivity equations (FSEs) by taking the partial derivative of FPDE with respect to q. These adjoint equations introduce a new fractional operator, associated with the logarithmic-power law kernel, which to best of our knowledge has been presented for the first time here in the context of fractional sensitivity analysis. The key property of derived FSEs is that they preserve the structure of original FPDE. Thus, similar discretization scheme and forward solver can be readily applied with a minimal required changes.

Model Construction: Estimation of Fractional Indices. Several numerical methods have been developed to solve inverse problem of model construction from available experimental observations or synthetic data. They typically convert the problem of model parameter estimation into an optimization problem, and then, formulate a suitable estimator by minimizing an objective function. These methods are stretched over but no limited to perturbation methods [60], weighted least squares approach [12, 15, 25], nonlinear regression [34], and Levenberg-Marquardt method [20, 13, 63, 64]. We develop a bi-level FSEM-based parameter estimation method in order to construct fractional models, in a sense that the method obtains model coefficients in one level, and then searches for estimate of fractional indices in the next level. We formulate the optimization problem by defining objective functions as two types of model error that measures the difference in computed output/input of fractional model with true output/input in an $L^2$-norm sense. We further formulate a gradient-based minimizer, employing developed FSEM, and propose a two-stage search algorithm, namely, coarse grid searching and nearby solution. The first stage construct a crude manifold of model error over a coarse discretization of parameter space to locate a local neighborhood of minimum, and the second stage uses the gradient decent method in order to converge to the minimum point.

Discretization Scheme. The iterative nature of parameter estimators instruct simulation of fractional model at each iteration step of model parameters. Therefore, one of the major tasks in computational model construction is to develop numerical methods that can efficiently discretize the physical domain and accurately solve the fractional model. The sensitivity framework additionally raise the complication by rendering coupled systems of FPDE and adjoint FSEs, and thus, demanding more versatile schemes. In addition to numerous finite difference methods [21, 54, 35, 57, 59, 11, 73, 71], recent works have elaborated efficient spectral schemes, for discretizing FPDEs in physical domain, see e.g., [46, 35, 26, 27, 32, 33, 14, 58, 7]. More recently, Zayernouri et al. [68, 66] developed two new spectral theories on fractional and tempered fractional Sturm-Liouville problems, and introduced explicit corresponding eigenfunctions, namely Jacobi poly-fractonomials of first and second kind. These eigenfunctions are comprised of smooth and fractional parts, where the latter can be tuned to capture singularities of true solution. They are successfully employed in constructing discrete solution/test function spaces and developing a series of high-order and efficient
Petrov-Galerkin spectral methods, see [70, 67, 69, 55, 49, 47, 30, 29, 28, 36, 50, 48]. We formulate a numerical scheme in solving coupled system of FPDE and adjoint FSEs by extending the mathematical framework in [49] and accommodating extra required regularity in the underlying function spaces. We employ Jacobi poly-fractonomials and Legendre polynomials as temporal and spatial basis/test functions, respectively, to develop a Petrov-Galerkin (PG) spectral method. The smart choice of coefficients in spatial basis/test functions yields symmetric property in the resulting mass/stiffness matrices, which is then exploited to formulate a fast solver. Following similar procedure as in [49], we also show that the coupled system is mathematically well-posed, and the proposed numerical scheme is stable.

The rest of paper is organized as follows. In section 2, we recall some preliminary definitions in fractional calculus and define proper solution/test spaces beside useful lemmas. In section 3, we define the problem by providing the fractional model, and then take the weak form of the problem as well. We develop FSEM in section 4 for the case of FIVP and FPDE. We define the underlying mathematical framework for the coupled system of FPDE and FSEs and also construct our Petrov-Galerkin spectral numerical scheme. Moreover, we formulate a numerical scheme in solving coupled system of FPDE and adjoint FSEs by extending the mathematical framework in [49] and accommodating extra required regularity in underlying function spaces. We employ Jacobi poly-fractonomials and Legendre polynomials as temporal and spatial basis/test functions, respectively, to develop a Petrov-Galerkin (PG) spectral method. The smart choice of coefficients in spatial basis/test functions yields symmetric property in the resulting mass/stiffness matrices, which is then exploited to formulate a fast solver. Following similar procedure as in [49], we also show that the coupled system is mathematically well-posed, and the proposed numerical scheme is stable.

2. Definitions. Let \( \xi \in [-1, 1] \). The left- and right-sided fractional derivative of order \( \sigma, n - 1 < \sigma \leq n, n \in \mathbb{N} \), are defined as (see e.g., [42, 45])

\[
(\frac{RL}{RL_D^\sigma}_\xi u)(\xi) = \frac{1}{\Gamma(n-\sigma)} \frac{d^n}{d\xi^n} \int_{-1}^{\xi} \frac{u(s)ds}{(\xi - s)^{1+\sigma}}, \quad \xi > -1,
\]

\[
(\frac{C}{C_D^\sigma}_\xi u)(\xi) = \frac{1}{\Gamma(n-\sigma)} (-1)^n \frac{d^n}{d\xi^n} \int_{\xi}^{1} \frac{u(s)ds}{(s-\xi)^{1+\sigma}}, \quad \xi < 1,
\]

respectively. An alternative approach in defining the fractional derivatives is the left- and right-sided Caputo derivatives of order \( \sigma \), defined as

\[
(\frac{C}{C_D^\sigma}_1 u)(\xi) = \frac{1}{\Gamma(n-\sigma)} \int_{-1}^{\xi} \frac{u^{(n)}(s)ds}{(\xi - s)^{1+\sigma}}, \quad \xi > -1,
\]

\[
(\frac{C}{C_D^\sigma}_1 u)(\xi) = \frac{1}{\Gamma(n-\sigma)} \int_{\xi}^{1} \frac{u^{(n)}(s)ds}{(s-\xi)^{1+\sigma}}, \quad \xi < 1.
\]

By performing an affine mapping from the standard domain \([-1, 1]\) to the interval \( t \in [a, b] \), we obtain

\[
\frac{RL}{RL_D^\sigma}_t u = \left(\frac{2}{b-a}\right)^\sigma (\frac{RL}{RL_D^\sigma}_1 u)(\xi),
\]

\[
\frac{C}{C_D^\sigma}_t u = \left(\frac{2}{b-a}\right)^\sigma (\frac{C}{C_D^\sigma}_1 u)(\xi).
\]

Hence, we can perform the operations in the standard domain only once for any given \( \sigma \) and efficiently utilize them on any arbitrary interval without resorting to repeating the calculations. Moreover, the corresponding relationship between the Riemann-Liouville and Caputo fractional derivatives in \([a, b]\) for any \( \sigma \in (0, 1) \) is given by

\[
(\frac{RL}{RL_D^\sigma}_t u)(t) = \frac{u(a)}{\Gamma(1-\sigma)(t-a)^\sigma} + (\frac{C}{C_D^\sigma}_t u)(t).
\]

**Definition 2.1.** We define the following left- and right-sided integro-differential operator with logarithmic-power law kernel, namely *Log-Pow integro-differential operator*, given as,
where $RL - LP$ and $C - LP$ stand for Log-Pow integro-differential operator, which partially resemble the fractional derivative in Riemann-Liouville and Caputo sense, respectively. The following lemma shows a useful relation between the two aforementioned operators.

**Lemma 2.2.** Let $x \in [a, b]$. Then, the following relation holds.

**Part A:** $\sigma \in (0, 1)$

\[
RL - LP_a D_x^\sigma u(x) = \frac{u(a)}{\Gamma(1 - \sigma)} \log(x - a) (x - a)^{-\sigma} + C - LP_a D_x^\sigma u(x).
\]

**Part B:** $\sigma \in (1, 2)$

\[
RL - LP_a D_x^\sigma u(x) = \frac{u(a)}{\Gamma(2 - \sigma)} \left(1 + (1 - \sigma) \log(x - a)\right) (x - a)^{\sigma - 1} + \frac{u'(a)}{\Gamma(2 - \sigma)} \log(x - a) (x - a)^{\sigma - 2} + C - LP_a D_x^\sigma u(x).
\]

**Proof.** See Appendix A for proof. □

### 2.1. Fractional Sobolev Spaces

We define some functional spaces and their associated norms [30, 32]. By $H^\sigma(\mathbb{R}) = \{u(t) | u \in L^2(\mathbb{R}); (1 + |\omega|^2)^{\frac{\sigma}{2}} \mathcal{F}(u)(\omega) \in L^2(\mathbb{R})\}$, $\sigma \geq 0$, we denote the fractional Sobolev space on $\mathbb{R}$, endowed with norm $|u|_{H^\sigma(\mathbb{R})} = ||(1 + |\omega|^2)^{\frac{\sigma}{2}} \mathcal{F}(u)(\omega)||_{L^2(\mathbb{R})}$, where $\mathcal{F}(u)$ represents the Fourier transform of $u$. Subsequently, we denote by $H^\sigma(\Lambda) = \{u \in L^2(\Lambda) | \exists \bar{u} \in H^\sigma(\mathbb{R}) \text{ s.t. } \bar{u}|_{\Lambda} = u\}$, $\sigma \geq 0$, the fractional Sobolev space on any finite closed interval, e.g. $\Lambda = (a, b)$, with norm $|u|_{H^\sigma(\Lambda)} = \inf_{\bar{u} \in H^\sigma(\mathbb{R})} ||\bar{u}||_{H^\sigma(\mathbb{R})}$. We define the following useful norms as:

\[
|\cdot|_{H^\sigma(\Lambda)} = \left(\|D_x^\sigma(\cdot)\|^2_{L^2(\Lambda)} + \|\cdot\|^2_{L^2(\Lambda)}\right)^{\frac{1}{2}},
\]

\[
|\cdot|_{H^\sigma(\Lambda)} = \left(\|D_x^\sigma(\cdot)\|^2_{L^2(\Lambda)} + \|\cdot\|^2_{L^2(\Lambda)}\right)^{\frac{1}{2}},
\]

\[
|\cdot|_{H^\sigma(\Lambda)} = \left(\|D_x^\sigma(\cdot)\|^2_{L^2(\Lambda)} + \|\cdot\|^2_{L^2(\Lambda)}\right)^{\frac{1}{2}}.
\]

where the equivalence of $|\cdot|_{H^\sigma(\Lambda)}$ and $|\cdot|_{H^\sigma(\Lambda)}$ are shown in [32, 19, 33]. We show the equivalence of these two norms with $|\cdot|_{H^\sigma(\Lambda)}$ in the following lemma.

**Lemma 2.3.** Let $\sigma \geq 0$ and $\sigma \neq n - \frac{1}{2}$. Then, the norms $|\cdot|_{H^\sigma(\Lambda)}$ and $|\cdot|_{H^\sigma(\Lambda)}$ are equivalent to $|\cdot|_{H^\sigma(\Lambda)}$.

**Proof.** See Appendix B for proof. □

We also define $C_0^\infty(\Lambda)$ as the space of smooth functions with compact support in $(a, b)$. We denote by $H^\sigma_0(\Lambda)$, $H^\sigma_0(\Lambda)$, and $H^\sigma_0(\Lambda)$ as the closure of $C_0^\infty(\Lambda)$ with respect to the norms $|\cdot|_{H^\sigma(\Lambda)}$, $|\cdot|_{H^\sigma(\Lambda)}$, and $|\cdot|_{H^\sigma(\Lambda)}$.

**Lemma 2.4 ([19, 33]).** The Sobolev spaces $H^\sigma_0(\Lambda)$, $H^\sigma_0(\Lambda)$, and $H^\sigma_0(\Lambda)$ are equal and their seminorms are equivalent to $|\cdot|_{H^\sigma(\Lambda)} = g\left(\frac{1}{2}ight)$.
Based on Lemma (2.4), and assuming that \( |\langle a, D^{\alpha}_{x} u, x D^{\beta}_{y} v \rangle_{\Lambda}| > 0 \) and \( |\langle a, D^{\alpha}_{x} u, x D^{\beta}_{y} v \rangle_{\Lambda}| > 0 \), we can prove that \( |\langle a, D^{\alpha}_{x} u, x D^{\beta}_{y} v \rangle_{\Lambda}| \geq \beta_1 \| u \|_{H^{\alpha}(\Lambda)} \| v \|_{H^{\beta}(\Lambda)} \) and \( |\langle a, D^{\alpha}_{x} u, x D^{\beta}_{y} v \rangle_{\Lambda}| \geq \beta_2 \| u \|_{H^{\alpha}(\Lambda)} \| v \|_{H^{\beta}(\Lambda)} \), where \( \beta_1 \) and \( \beta_2 \) are positive constants. Following [49], we define the corresponding solution and test spaces of our problem. Thus, by letting \( \Lambda_j = (a_1, b_1), \Lambda_j = (a_j, b_j) \times \Lambda_{j-1} \) for \( j = 2, \cdots, d \), we define \( \mathcal{X}_j = H^{\frac{p}{2}}_0(\Lambda_j), \) which is associated with the norm \( \| \cdot \|_{H^{\frac{p}{2}}(\Lambda_j)} \), and accordingly, \( \mathcal{X}_j, j = 2, \cdots, d \) as

\[
\mathcal{X}_2 = H^{\frac{p}{2}}_0((a_2, b_2); L^2(\Lambda_1)) \cap L^2((a_2, b_2); \mathcal{X}_1),
\]

\[
\mathcal{X}_d = H^{\frac{p}{2}}_0((a_d, b_d); L^2(\Lambda_d-1)) \cap L^2((a_d, b_d); \mathcal{X}_{d-1}),
\]

associated with norms \( \| \cdot \|_{\mathcal{X}_j} = \left( \| \cdot \|_{H^{\frac{p}{2}}_0((a, b); L^2(\Lambda_{j-1}))}^2 + \| \cdot \|_{L^2((a, b); \mathcal{X}_{j-1})}^2 \right)^{\frac{1}{2}}, \) \( j = 2, 3, \cdots, d. \)

**Lemma 2.5.** Let \( \sigma \geq 0 \) and \( \sigma \neq n - \frac{1}{2} \). Then, for \( j = 1, 2, \cdots, d \)

\[
\| \cdot \|_{\mathcal{X}_j} = \sum_{i=0}^{j} \left( \| x D^{\beta}_{x} (\cdot) \|^2_{L^2(\Lambda_j)} + \| a_0 D^{\beta}_{y} (\cdot) \|^2_{L^2(\Lambda_j)} \right)^{\frac{1}{2}}, \quad j = 1, 2, \cdots, d.
\]

**Proof.** See Appendix C for proof.

Moreover, by letting \( o^{C^\infty}(I) \) and \( C^\infty_0(I) \) be the space of smooth functions with compact support in \( (0, T) \) and \( [0, T) \), respectively, we define \( \mathcal{H}^H(I) \) and \( \mathcal{H}^T(I) \) as the closure of \( C^\infty_0(I) \) and \( C^\infty_0(I) \) with respect to the norms \( \| \cdot \|_{H^H(I)} \) and \( \| \cdot \|_{H^T(I)} \). We also define

\[
o^{\mathcal{H}}^T(I; L^2(\Lambda_{d})) = \left\{ u \left| \begin{array}{l}
\| u(t, \cdot) \|_{L^2(\Lambda)} \in H^T(I), u|_{t=0} = u|_{x=a_j} = u|_{x=b_j} = 0, j = 1, 2, \cdots, d,
\end{array} \right. \right\},
\]

\[
o^{\mathcal{H}}^T(I; L^2(\Lambda_{d})) = \left\{ v \left| \begin{array}{l}
\| v(t, \cdot) \|_{L^2(\Lambda)} \in H^T(I), v|_{t=0} = v|_{x=a_j} = v|_{x=b_j} = 0, j = 1, 2, \cdots, d,
\end{array} \right. \right\},
\]

equipped with norms \( \| u \|_{H^T(I; L^2(\Lambda_{d}))} \) and \( \| u \|_{H^T(I; L^2(\Lambda_{d}))} \), respectively, which take the following forms

\[
\| u \|_{H^T(I; L^2(\Lambda_{d}))} = \left( \| u(t, \cdot) \|^2_{L^2(\Lambda)} + \| u \|^2_{L^2(\Lambda)} \right)^{\frac{1}{2}},
\]

\[
\| u \|_{H^T(I; L^2(\Lambda_{d}))} = \left( \| u(t, \cdot) \|^2_{L^2(\Lambda)} + \| u \|^2_{L^2(\Lambda)} \right)^{\frac{1}{2}}.
\]

**Solution and Test Spaces.** We define the solution space \( U \) and test space \( V \), respectively, as

\[
U = o^{H^T(I; L^2(\Lambda_{d}))} \cap L^2(I; \mathcal{X}_d), \quad V = o^{H^T(I; L^2(\Lambda_{d}))} \cap L^2(I; \mathcal{X}_d),
\]

endowed with norms

\[
\| u \|_U = \left( \| u \|^2_{H^T(I; L^2(\Lambda_{d}))} + \| u \|^2_{L^2(\Lambda_{d})} \right)^{\frac{1}{2}}, \quad \| v \|_V = \left( \| v \|^2_{H^T(I; L^2(\Lambda_{d}))} + \| v \|^2_{L^2(\Lambda_{d})} \right)^{\frac{1}{2}}.
\]

Using Lemma 2.5, we can show that

\[
\| u \|_{L^2(I; \mathcal{X}_d)} = \left( \| u(t, \cdot) \|^2_{L^2(\Lambda)} + \left( \| u \|^2_{L^2(\Lambda)} + \sum_{j=1}^{d} \| a_0 D^{\beta}_{y} u \|^2_{L^2(\Lambda)} + \| a_0 D^{\beta}_{y} u \|^2_{L^2(\Lambda)} \right)^{\frac{1}{2}}.
\]
Therefore, by (2.16) we write (2.19) as

\begin{equation}
\|u\|_V = \left\{ \|u\|_{L^2(\Omega)}^2 + \|\partial_\alpha \partial_0^{\beta_j} u\|_{L^2(\Omega)}^2 + \sum_{j=1}^{d} (\|\partial_\alpha \partial_0^{\beta_j} u\|_{L^2(\Omega)}^2 + \|\partial_\alpha \partial_0^{\beta_j} u\|_{L^2(\Omega)}^2) \right\}^{1/2},
\end{equation}

(2.21)

\begin{equation}
\|v\|_V = \left\{ \|v\|_{L^2(\Omega)}^2 + \|\partial_\alpha \partial_0^{\beta_j} v\|_{L^2(\Omega)}^2 + \sum_{j=1}^{d} (\|\partial_\alpha \partial_0^{\beta_j} v\|_{L^2(\Omega)}^2 + \|\partial_\alpha \partial_0^{\beta_j} v\|_{L^2(\Omega)}^2) \right\}^{1/2},
\end{equation}

(2.22)

The following lemmas help us obtain the weak formulation of our problem, construct the numerical scheme and further prove the stability of our method.

**Lemma 2.6.** [32]: For all \( \alpha \in (0, 1) \), if \( u \in H^1([0, T]) \) such that \( u(0) = 0 \), and \( v \in H^{\alpha/2}([0, T]) \), then \( \langle \partial_0^{\alpha/2} u, v \rangle_\Omega = \langle \partial_0^{\alpha/2} u, \partial_0^{\alpha/2} v \rangle_\Omega \), where \( \langle \cdot, \cdot \rangle_\Omega \) represents the standard inner product in \( \Omega = [0, T] \).

**Lemma 2.7.** [30]: Let \( 1 < \beta < 2 \), and \( a \) and \( b \) be arbitrary finite or infinite real numbers. Assume \( u \in H^\beta(a, b) \) such that \( u(a) = 0 \), then \( \partial_\alpha \partial_0^{\beta_j} v \) is integrable in \( \Omega = (a, b) \) such that \( v(b) = 0 \). Then, \( \partial_\alpha \partial_0^{\beta_j} u, v \rangle_\Omega = \langle \partial_\alpha \partial_0^{\beta_j} u, x_\alpha \partial_0^{\beta_j} v \rangle_\Omega \).

We generalize Lemma 2.7 to the two-sided \((1 + d)\)-dimensional case (see Appendix D for proof).

**Lemma 2.8.** Let \( 1 < \beta_j < 2 \) for \( j = 1, 2, \ldots, d \), and \( u, v \in X_d \). Then,

\[
\langle \partial_\alpha \partial_0^{\beta_j} u, v \rangle_\Omega = \langle \partial_\alpha \partial_0^{\beta_j} u, x_\alpha \partial_0^{\beta_j} v \rangle_\Omega, \quad \langle x_\alpha \partial_0^{\beta_j} u, v \rangle_\Omega = \langle x_\alpha \partial_0^{\beta_j} u, x_\alpha \partial_0^{\beta_j} v \rangle_\Omega.
\]

**3. Problem Definition.** Let \( \Omega = (0, T] \times (a_1, b_1) \times (a_2, b_2) \times \cdots \times (a_d, b_d) \) be the computational domain for some positive integer \( d \). We define \( u(t, x; q) : \Omega \times Q \rightarrow \mathbb{R} \), where \( q = \{\alpha, \beta_1, \beta_2, \ldots, \beta_d, k_1, k_2, \ldots, k_d\} \) is the vector of model parameters containing the fractional indices and model coefficients, and \( Q = [0, 1]^d \times \mathbb{R}^d \) is the space of parameters. Thus, for any \( q \in Q \), the transport field \( u(t, x; q) : \Omega \rightarrow \mathbb{R} \). We consider the FPDE of strong form \( \mathcal{L}(u) = f \), subject to Dirichlet initial and boundary conditions, where \( \mathcal{L} \) is a linear two-sided fractional operator, given as follows

\begin{equation}
0 \partial_\alpha \partial_0^{\beta_j} u(t, x; q) - \sum_{j=1}^{d} k_j \left[ \partial_\alpha \partial_0^{\beta_j} u + x_\alpha \partial_0^{\beta_j} v \right] u(t, x; q) = f(t, x; q),
\end{equation}

(3.1)

\begin{equation}
|u|_{t=0} = 0,
\end{equation}

(3.2)

\begin{equation}
|u|_{x=a_j} = |u|_{x=b_j} = 0,
\end{equation}

(3.3)

in which \( \alpha \in (0, 1) \), \( \beta_j \in (1, 2) \), \( k_j \) are real positive constant coefficients, and the fractional derivatives are taken in the Riemann-Liouville sense.

**3.1. Weak Formulation.** For any set of model parameter \( q \), we obtain the weak system, i.e. the variational form of the problem (3.1) subject to the given initial/boundary conditions, by multiplying the equation with proper test functions and integrate over the whole computational domain \( \Omega \). Therefore, using Lemmas 2.6-2.8, the bilinear form can be written as

\begin{equation}
a(u, v) = \langle 0 \partial_\alpha \partial_0^{\beta_j} u, \partial_\alpha \partial_0^{\beta_j} v \rangle_\Omega - \sum_{j=1}^{d} k_j \left[ \langle \partial_\alpha \partial_0^{\beta_j} u, x_\alpha \partial_0^{\beta_j} v \rangle_\Omega + \langle x_\alpha \partial_0^{\beta_j} u, \partial_\alpha \partial_0^{\beta_j} v \rangle_\Omega \right],
\end{equation}

(3.4)

and thus, by letting \( \bar{U} \) and \( \bar{V} \) be the proper solution/test spaces, the problem reads as: find \( u \in \bar{U} \) such that

\begin{equation}
a(u, v) = (f, v)_\Omega, \quad \forall v \in \bar{V}.
\end{equation}

(3.5)
4. Fractional Sensitivity Equation Method (FSEM). We define the sensitivity coefficients as the partial derivative of transport field $u$ with respect to the model parameters $q_i$, i.e.

$$(4.1) \quad S_{u,q_i} = \frac{\partial u}{\partial q_i}, \quad i = 1, 2, \cdots, 2d + 1,$$

assuming that the partial derivative is well-defined. To obtain the governing equation of evolution of sensitivity fields, i.e. FSEs, we first take the partial derivative of left- and right-sided fractional derivative (2.1) and (2.2) with respect to their orders. Therefore, by letting $\sigma \in (n - 1, n]$, $x \in [a, b]$, $\mathcal{A}_n(\sigma) = \Gamma(n - \sigma) \frac{\Gamma(n - \sigma)}{\Gamma(\sigma)}$, we have

$$(4.2) \quad \frac{\partial}{\partial \sigma} (D^\sigma_x u) = D^\sigma_x S_{u,\sigma} + \mathcal{A}_n(\sigma) \frac{\partial}{\partial \sigma} (D^\sigma_x u) - L^\sigma_x D^\sigma_x u,$$

$$(4.3) \quad \frac{\partial}{\partial \sigma} (D^\sigma_u u) = D^\sigma_u S_{u,\sigma} + \mathcal{A}_n(\sigma) \frac{\partial}{\partial \sigma} (D^\sigma_u u) - L^\sigma_u D^\sigma_u u.$$

The pre-super script LP stands for the Log-Pow integro-differential operator, given in (2.8)-(2.11), which we introduce here, for the first time in the context of FSEs.

**Remark 4.1.** In the sequel, we only use the RL – LP operator and thus, for the sake of simplicity, we drop the pre-super script RL and C and only use them when needed to distinguish between the two senses of derivatives.

We derive the adjoint FSEs by pursuing two different strategies I and II, shown schematically in Fig. 1. We adopt the notation of $u'$ and $u''$ to distinguish the solution to strong and weak form of the problem for ease of describing the two following strategies. In the first strategy, we first take the partial derivative of FPDE with respect to the model parameters $q$, and then, obtain the weak form of problem. If $u'$ is known, then we follow I-1 (left figure), otherwise we formulate and solve the weak form of FPDE to obtain weak solution $u''$ and follow I-2 (middle figure).

$$(4.4) \quad \text{I-1: } \mathcal{L}^i(u') = f \xrightarrow{\text{weak form}} \mathcal{L}^i(S_{u',q_i}^\sigma) = f_q(u') \xrightarrow{\text{weak form}} a(S_{u',q_i}^\sigma, v) = (f_q(u'), v)_{\Omega}$$

$$(4.5) \quad \text{I-2: } \mathcal{L}^i(u') = f \xrightarrow{\text{weak form}} \mathcal{L}^i(S_{u',q_i}^\sigma) = f_q(u') \xrightarrow{\text{weak form}} a(S_{u',q_i}^\sigma, v) = (f_q(u''), v)_{\Omega}$$

Fig. 1: Schematic of strategies in deriving the weak form of FSEs. (I-1): first take $\frac{\partial}{\partial q}$ and then obtain the weak formulation, fed by strong solution $u'$. (I-2): first take $\frac{\partial}{\partial q}$ and then obtain the weak formulation, fed by weak solution $u''$. (II): first obtain the weak formulation and then take $\frac{\partial}{\partial q}$, fed by weak solution $u''$. 
Via proper construction of the corresponding subspaces, we discretize and solve \(a(S_{w,q}^u, v) = (f_q(u^w), v)_{\Omega} \) and \(a(S_{w,q}^v, v) = (f_q(u^v), v)_{\Omega} \) in I-1 and I-2, respectively. We can show that \(\|S_{w,q}^v - S_{w,q}^u\|_L^2 \to 0\) as \(u^v \to u^w\) by stability/error analysis of employed numerical scheme, where the solution space has the extra regularity required by the Log-Pow integro-differential operator in \(f_q\).

**Remark 4.2.** The solution to strong form of FPDE, i.e. \(u^w\) can be analytically/numerically computed (by Laplace transform and finite difference method for example), or may be available as prior experimental data, and thus, can be fed directly to construct \(f_q\) in FSEs (see left sub-figure in Fig. 1). This is used in parameter estimation for model construction, section 5.

In the second strategy, we first obtain the weak form of FPDE, and then take the partial derivative with respect to the model parameters \(q\). In this case, we procure \((h(u^w), v)\) as the right hand side of weak formulation, which is fed by the weak solution \(u^w\). In this case, \(h\) requires less regularity for the solution space due to the Log-Pow integro-differential operator, since the order of kernel is less compare to the first strategy.

\[
\text{(4.6) II: } L^i(u^w) = f \quad \xrightarrow{\text{weak form}} \quad a(u^w, v) = (f, v)_{\Omega} \quad \frac{\partial}{\partial \alpha} a(S_{w,q}^u, v) = (h(u^w), v)_{\Omega}
\]

In the next subsection, we adopt the two strategies to derive adjoint FSE to a fractional initial value problem, where we show the corresponding right-hand-side and the imposed extra regularity in each case. We then, extend the derivation to the case FPDE, in which we adopt strategy I-2.

### 4.1. FSEM (FIVP)

Let \(\Omega = (0, T]\) be the computational domain and define \(u(t; \alpha) : \Omega \times (0, 1) \to \mathbb{R}\). We consider the case of fractional initial value problem (FIVP) by letting the coefficients \(k_j\)'s to be zero in (3.1), and thus obtain the following FIVP, subject to Dirichlet initial condition, as \(\alpha \partial_0^\alpha D_\alpha^\beta u(t; \alpha) = f(t; \alpha), u(0) = 0\). By taking the partial derivative with respect to \(\alpha\), we obtain the adjoint FSE in the strong form as \(\alpha \partial_0^\alpha D_\alpha^\beta S_{\alpha,\alpha} = f_{\alpha}, S_{\alpha,\alpha}|_{t=0} = 0\), where \(f_{\alpha} = S_{f,\alpha} - A_1(\alpha) \partial_0^\alpha D_\alpha^\beta u + \partial_0^\alpha D_\alpha^\beta \). Following strategy I, we obtain

\[
\text{(4.7) } a(S_{\alpha,\alpha}, v)_{\Omega} = (f_{\alpha}, v)_{\Omega}
\]

\[
\text{(4.8) } (f_{\alpha}, v)_{\Omega} = (S_{f,\alpha}, v)_{\Omega} - A_1(\alpha) (\alpha \partial_0^\alpha D_\alpha^\beta u, \partial_0^\alpha D_\alpha^\beta v)_{\Omega} + (\partial_0^\alpha D_\alpha^\beta u, v)_{\Omega}.
\]

In this case, constructing the right-hand-side imposes extra strong regularity of \(\|\partial_0^\alpha D_\alpha^\beta u\|_L^2 < \infty\) to the solution of FIVP. However, by following startegy II, we obtain

\[
\text{(4.9) } a(S_{\alpha,\alpha}, v)_{\Omega} = h(v),
\]

\[
\text{(4.10) } h(v) = (S_{f,\alpha}, v)_{\Omega} + (f, v)_{\Omega} - A_1(\alpha) \left(\frac{\alpha}{2} (\partial_0^\alpha D_\alpha^\beta u, \partial_0^\alpha D_\alpha^\beta v)_{\Omega} - (\partial_0^\alpha D_\alpha^\beta u, \partial_0^\alpha D_\alpha^\beta v)_{\Omega}ight) + \frac{1}{2} (\partial_0^\alpha D_\alpha^\beta u, \partial_0^\alpha D_\alpha^\beta v)_{\Omega} + \frac{1}{2} (\partial_0^\alpha D_\alpha^\beta u, \partial_0^\alpha D_\alpha^\beta v)_{\Omega},
\]

where, the function \(h\) imposes extra weak regularity of \(\|\partial_0^\alpha D_\alpha^\beta u\|_L^2 < \infty\) and \(\|\partial_0^\alpha D_\alpha^\beta v\|_L^2 < \infty\) to the solution. We computationally study and make sure that the solution to (4.7) converges to (4.9).

### 4.2. FSEM (FPDE)

We consider the problem (3.1)-(3.3). We adopt strategy I-2 and derive the adjoint FSEs and their corresponding weak form, where to construct the right-hand-side, we also obtain the weak form of FPDE. Thus, we solve a coupled system of FPDE and FSEs. By taking the partial derivatives of (3.1) with respect to model parameters \(q_i, i =

We extend the solution (4.11) associated with the similar norm (4.18) and "test space" \( \tilde{U} \), respectively, as

\[
\mathcal{X}_i = \mathcal{H}_0^{\bar{p}_i}((a_i, b_i); L^2(\mathcal{A}_i)) \cap L^2((a_i, b_i); \mathcal{X}_1),
\]

associated with the similar norm \( \| \cdot \|_{\mathcal{H}_0^{\bar{p}_i}(\mathcal{A}_i)} \). We define \( \mathcal{X}_1 = \mathcal{H}_0^{\bar{p}_1}(\mathcal{A}_1) \), and accordingly, \( \mathcal{X}_j, j = 2, \cdots, d \) as

\[
\mathcal{X}_1 = \mathcal{H}_0^{\bar{p}_1}(\mathcal{A}_1) \cap L^2(\mathcal{A}_1),
\]

\[
\mathcal{X}_d = \mathcal{H}_0^{\bar{p}_d}(\mathcal{A}_d) \cap L^2(\mathcal{A}_d),
\]

associated with the similar norm \( \| \cdot \|_{\mathcal{X}_i} \). Thus, we define the corresponding "solution space" \( \tilde{U} \) and "test space" \( \tilde{V} \), respectively, as

\[
\tilde{U} = \mathcal{H}^{\mathcal{X}}(I; L^2(\mathcal{A}_d)) \cap L^2(I; \mathcal{X}_d),
\]

\[
\tilde{V} = \mathcal{H}^{\mathcal{X}}(I; L^2(\mathcal{A}_d)) \cap L^2(I; \mathcal{X}_d),
\]

endowed with similar norms (2.21) and (2.22), where

\[
\mathcal{H}^{\mathcal{X}}(I; L^2(\mathcal{A}_d)) = \{ u \mid \| u(t, \cdot) \|_{L^2(\mathcal{A}_d)} \in H^{\mathcal{X}}(I), \| L_{\mathcal{A}_d}^{\bar{p}_d} u \|_{L^2(\mathcal{A}_d)} < \infty, u|_{t=0} = u|_{t=b} = 0, j = 1, 2, \cdots, d \}
\]

\[
\mathcal{H}^{\mathcal{X}}(I; L^2(\mathcal{A}_d)) = \{ v \mid \| v(t, \cdot) \|_{L^2(\mathcal{A}_d)} \in H^{\mathcal{X}}(I), \| L_{\mathcal{A}_d}^{\bar{p}_d} v \|_{L^2(\mathcal{A}_d)} < \infty, v|_{t=0} = v|_{t=b} = 0, j = 1, 2, \cdots, d \}
\]
Weak Formulation. Since derived FSEs (4.11) preserve the structure of FPDE (3.1), the bilinear form of corresponding weak formulation takes the same form as (3.4). Therefore, By letting \( \tilde{U} \) and \( \tilde{V} \) be the solution/test spaces, defined in (4.19), the problem reads as: find \( u \in \tilde{U} \) such that

\[
(4.20) \quad a(u, v) = (f, v)_{\Omega}, \quad \forall v \in \tilde{V},
\]

and find \( S_{a,q} \in U, \quad 1 = 1, 2, \cdots , 2d + 1 \) such that

\[
(4.21) \quad a(S_{a,q}, w) = (f_q, w)_{\Omega} \quad \forall w \in V,
\]

where \( U \) and \( V \) are defined in (2.18).

4.4. Petrov-Galerkin Spectral Method. We define the following finite dimensional solution and test spaces. We employ Legendre polynomials \( \phi_m(\xi), \quad j = 1, 2, \cdots , d \), and Jacobi poly-fractonomial of first kind \( \psi_n^\tau(\eta) \) [66, 68], as the spatial and temporal bases, respectively, given in their corresponding standard domain as

\[
(4.22) \quad \phi_m(\xi) = \sigma_m(P_m+1(\xi) - P_m-1(\xi)), \quad \xi \in [-1, 1] \quad m_j = 1, 2, \cdots ,
\]

\[
(4.23) \quad \psi_n^\tau(\eta) = \sigma_n^{(1)}P_n^\tau(\eta) = \sigma_n(1 + \eta)P_n^{\tau^-}(\eta), \quad \eta \in [-1, 1] \quad n = 1, 2, \cdots ,
\]

in which \( \sigma_m = 2 + (-1)^m \). Therefore, by performing affine mappings \( \eta = 2^\tau - 1 \) and \( \xi = 2^{\frac{a}{a_1 - a_i}} - 1 \) from the computational domain to the standard domain, we construct the solution space \( U_N \) as

\[
(4.24) \quad U_N = \text{span} \left\{ \left( \psi_n^\tau \circ \eta \right)(t) \prod_{j=1}^{d} \left( \phi_m \circ \xi \right)(x_j) : n = 1, 2, \cdots , N, \quad m_j = 1, 2, \cdots , M_j \right\}.
\]

We note that the choice of temporal and spatial basis functions naturally satisfy the initial and boundary conditions, respectively. The parameter \( \tau \) in the temporal basis functions plays a role of fine tuning parameter, which can be chosen properly to capture the singularity of exact solution.

Moreover, we employ Legendre polynomials \( \Phi_j(\xi), \quad j = 1, 2, \cdots , d \), and Jacobi poly-fractonomial of second kind \( \Psi_k^\tau(\eta) \), as the spatial and temporal test functions, respectively, given in their corresponding standard domain as

\[
(4.25) \quad \Phi_j(\xi) = \bar{\sigma}_j(P_{j+1}(\xi) - P_{j-1}(\xi)), \quad \xi \in [-1, 1] \quad r_j = 1, 2, \cdots ,
\]

\[
(4.26) \quad \Psi_k^\tau(\eta) = \bar{\sigma}_k^{(2)}(1 - \eta)^{\tau}P_{k-1}^{\tau^-}(\eta), \quad \eta \in [-1, 1] \quad k = 1, 2, \cdots ,
\]

where \( \bar{\sigma}_j = 2(-1)^{r_j} + 1 \). Therefore, by similar affine mapping we construct the test space \( V_N \) as

\[
(4.27) \quad V_N = \text{span} \left\{ \left( \Psi_k^\tau \circ \eta \right)(t) \prod_{j=1}^{d} \left( \Phi_j \circ \xi \right)(x_j) : k = 1, 2, \cdots , N, \quad r_j = 1, 2, \cdots , M_j \right\}.
\]

We can show that our choice of basis/test functions satisfy the extra regularity imposed by the Log-Pow integro-differential operator. Thus, since \( U_N \subset \tilde{U} \subset U \) and \( V_N \subset \tilde{V} \subset V \), the problems (4.20) and (4.21) read as: find \( u_N \in U_N \) such that

\[
(4.28) \quad a_h(u_N, v_N) = l(v_N), \quad \forall v_N \in V_N,
\]
where \( l(v_N) = (f, v_N) \); and find \( S u_N \in U_N \) such that

\[
a_h(S u_N, w_N) = l(w_N), \quad \forall w_N \in V_N,
\]

where \( l(w_N) = (f_N, w_N) \). Also, the discrete bilinear form \( a_h(u_N, v_N) \) can be written as

\[
a_h(u_N, v_N) = (a \mathcal{D}_r^2 u_N, \mathcal{D}_r^2 v_N)_{\Omega} - \sum_{j=1}^d k_j \left[ \left( \mathcal{D}_r^2 u_N, \mathcal{D}_r^2 v_N \right)_{\Omega} + (x, \mathcal{D}_r^2 u_N, a_j \mathcal{D}_r^2 v_N)_{\Omega} \right].
\]

We expand the approximate solution \( u_N \in U_N \), satisfying the discrete bilinear form (4.30), in the following form

\[
u_N(t, x) = \sum_{n=1}^N \sum_{m_1=1}^{M_1} \cdots \sum_{m_d=1}^{M_d} \hat{u}_{n,m_1,\ldots,m_d} \left[ \psi_n(t) \prod_{j=1}^d \phi_{m_j}(x_j) \right],
\]

and obtain the corresponding Lyapunov system by substituting (4.31) into (4.30) by choosing \( v_N(t, x) = \Psi_n(t) \prod_{j=1}^d \Phi_{m_j}(x_j), \quad k = 1, 2, \ldots, N, \quad r_j = 1, 2, \ldots, M_j \). Therefore,

\[
\begin{align*}
S_T \otimes M_1 \otimes M_2 \cdots \otimes M_d &+ \sum_{j=1}^d M_T \otimes M_1 \otimes \cdots \otimes M_{j-1} \otimes S_T^{tot} \otimes M_{j+1} \cdots \otimes M_d \\
&+ \gamma M_T \otimes M_1 \otimes M_2 \cdots \otimes M_d \right) \mathcal{U} = F,
\end{align*}
\]

in which \( \otimes \) represents the Kronecker product, \( F \) denotes the multi-dimensional load matrix whose entries are given as

\[
F_{k,r_1,\ldots,r_d} = \int_{\Omega} f(t, x) \left( \Psi_k(t) \circ \eta \right) \prod_{j=1}^d \left( \Phi_{r_j} \circ \xi_j \right)(x_j) \, d\Omega,
\]

and \( \mathcal{U} \) is the matrix of unknown coefficients. The matrices \( S_T \) and \( M_T \) denote the temporal stiffness and mass matrices, respectively; and the matrices \( S_j \) and \( M_j \) denote the spatial stiffness and mass matrices, respectively. We obtain the entries of spatial mass matrix \( M_j \) analytically and employ proper quadrature rules to accurately compute the entries of other matrices \( S_T, M_T \) and \( S_j \).

We note that the choices of basis/test functions, employed in developing the PG scheme leads to symmetric mass and stiffness matrices, providing useful properties to further develop a fast solver. The following Theorem 4.3 provides a unified fast solver, developed in terms of the generalized eigensolutions in order to obtain a closed-form solution to the Lyapunov system (4.32).

**Theorem 4.3 (Unified Fast FPDE Solver [49, 47]).** Let \( \{ \tilde{v}_n^\mu, \lambda_{m_j}^{M_j} \}_{j=1}^{M_j} \) be the set of general eigen-solutions of the spatial stiffness matrix \( S_T^{tot} \) with respect to the mass matrix \( M_j \). Moreover, let \( \{ \tilde{v}_n^r, \lambda_j^{M_T} \}_{r=1}^{M_T} \) be the set of general eigen-solutions of the temporal mass matrix \( M_T \) with respect to the stiffness matrix \( S_T \). Then, the matrix of unknown coefficients \( \mathcal{U} \) is explicitly obtained as

\[
\mathcal{U} = \sum_{n=1}^N \sum_{m_1=1}^{M_1} \cdots \sum_{m_d=1}^{M_d} \kappa_{n,m_1,\ldots,m_d} \tilde{v}_n^\mu \otimes \tilde{v}_m^r \otimes \cdots \otimes \tilde{v}_{m_d},
\]
where $\kappa_{n,m_1,\ldots,m_d}$ is given by
\[
\kappa_{n,m_1,\ldots,m_d} = \frac{\langle S T \bar{e}_n, \prod_{j=1}^d (\bar{e}_{m_j} M_j \bar{e}_{m_j}), \Lambda_{n,m_1,\ldots,m_d} \rangle}{\langle \bar{e}_n, S T \bar{e}_n \rangle},
\]
in which the numerator represents the standard multi-dimensional inner product, and $\Lambda_{n,m_1,\ldots,m_d}$ is obtained in terms of the eigenvalues of all mass matrices as
\[
\Lambda_{n,m_1,\ldots,m_d} = \left[ (1 + \gamma A_n^2) + \lambda_n^2 \sum_{j=1}^d (\Lambda_{m_j}) \right].
\]

### 4.5. Stability Analysis

We show the well-posedness of defined problem and prove the stability of proposed scheme.

**Lemma 4.4.** Let $\alpha \in (0, 1)$, $\Omega = I \times \Lambda_d$, and $u \in H^{\frac{\alpha}{2}}(L^2(\Lambda_d))$. Then,
\[
\left| \langle \mathcal{D}_d^{\alpha/2} u, \mathcal{D}_d^{\alpha/2} v \rangle \right| \leq ||u||_{H^{\alpha/2}(L^2(\Lambda_d))} ||v||_{H^{\alpha/2}(L^2(\Lambda_d))}, \quad \forall v \in H^{\alpha/2}(L^2(\Lambda_d)).
\]

**Proof.** See Appendix E for proof.

By equivalence of function spaces $H^{\alpha}(\Lambda)$, $H^{\alpha}(\Lambda)$, and $H_{m}^{\alpha}(\Lambda)$ and also their associated norms $\|u\|_{H^{\alpha}(\Lambda)}$, $\|u\|_{H^{\alpha}(\Lambda)}$, and $\|u\|_{H^{\alpha}(\Lambda)}$; and also by following similar steps as in Lemma 4.4, we can also prove that
\[
\left| \langle \mathcal{D}_d^{\alpha/2} u, \mathcal{D}_d^{\alpha/2} v \rangle \right| \leq ||u||_{H^{\alpha/2}(L^2(\Lambda_d))} ||v||_{H^{\alpha/2}(L^2(\Lambda_d))}, \quad \forall v \in H^{\alpha/2}(L^2(\Lambda_d)).
\]

**Lemma 4.5 (Continuity).** The bilinear form (3.4) is continuous, i.e.,
\[
\inf_{u \neq 0 \in U} \sup_{v \neq 0 \in V} \frac{|a(u,v)|}{||u||_V ||v||_U} \geq \beta > 0,
\]
where $\Omega = I \times \Lambda_d$ and $\inf_{u \neq 0 \in U} \sup_{v \neq 0 \in V} |a(u,v)| > 0$.

**Proof.** See Appendix F for proof.

**Theorem 4.6 (Stability).** The following inf-sup condition holds for the bilinear form (3.4), i.e.,
\[
\inf_{u \neq 0 \in U} \sup_{v \neq 0 \in V} \frac{|a(u,v)|}{||u||_V ||v||_U} \geq \beta > 0,
\]

where $\Omega = I \times \Lambda_d$.}

**Proof.** The proof directly concludes from (4.36), (4.37) and Lemma 4.4.

**Theorem 4.7 (well-posedness).** For all $0 < \alpha < 1$, $\alpha \neq 1$, and $1 < \beta_j < 2$, and $j = 1, \ldots, d$, there exists a unique solution to (3.5), continuously dependent on $f$, which belongs to the dual space of $U$.

**Proof.** Lemmas 4.5 (continuity) and 4.6 (stability) yield the well-posedness of weak form (3.5) in (1+d) dimension due to the generalized Babuška-Lax-Milgram theorem.

Since the defined basis and test spaces are Hilbert spaces, and $U_N \subset U$ and $V_N \subset V$, we can prove that the developed Petrov-Galerkin spectral method is stable and the following condition holds
\[
\inf_{0 \neq u \in U_N} \sup_{0 \neq v \in V_N} \frac{|a(u_N,v_N)|}{||v_N||_V ||u_N||_U} \geq \beta > 0,
\]
5. Fractional Model Construction. We employ the developed FSEM in order to construct an iterative algorithm to estimate model parameters from known solution (or available sets of data). We formulate the iterative algorithm by minimizing an objective model error function. We recall again here that in our fractional model, the set of model parameters is \( q = \{ \alpha, \beta_1, \beta_2, \cdots, \beta_d, k_1, k_2, \cdots, k_d \} \), and here, we mainly focus on estimation of fractional indices. Thus, assuming the model coefficients \( \{ k_1, k_2, \cdots, k_d \} \) to be given/known, we reduce the model parameter set to \( q = \{ \alpha, \beta_1, \beta_2, \cdots, \beta_d \} \in Q \subset \mathbb{R}^{1+d} \).

5.1. Model Error. The fractional model can be simply visualized as Fig. 2, where \( L^q u = f \). We denote by the superscript \((\ast)\) as the exact values of quantities. Therefore, \( L^q u^\ast = f^\ast \), where \( u^\ast, f^\ast \) are the exact solution and force functions, respectively, and \( q^\ast \) is the set of exact model parameters. Obviously, by choosing different values of model parameters (fractional indices), the fractional model observes the input differently, and thus, results in a different output. This leads to two types of model error, namely, type-I and type-II, described as follows. We note that the introduced model errors are zero at the exact values \( q^\ast \), by definition.

5.1.1. Model Error: Type-I. In model error type-I, we consider the output of model to be fixed, i.e., \( f = f^\ast \), however, changing parameters makes the fractional model to observe the variated input \( u^q \) as opposed to \( u^\ast \). Therefore, we define the model error as the difference between variated and exact inputs, i.e., \( E(q) = \|u^q - u^\ast\|_{L^2} \). The schematic of variation of model from the exact model is shown in Fig. 3 (a). For each variated model, we accurately compute the numerical approximation, \( u^q_N \), by solving (3.1), where by increasing the number of terms in the approximate solution, we make sure that the function \( E(q) = \|u^q_N - u^\ast\|_{L^2} \) solely describes the model error with minimum discretization error. The proposed iterative algorithm, as will be discussed later, involves the gradient of model error with respect to the model parameters. Thus, we take the partial derivative of \( E \) with respect to \( q \), as

\[
S_{E,q} = \frac{\partial E}{\partial q} = \int_{\Omega} S_{u^q} (u^q_N - u^\ast) \, d\Omega
\]  

(5.1)
where $S_{u,q}$ denotes the sensitivity fields, which is numerically obtained by solving FSEs (4.11). We note that in this case, since $f$ is fixed and therefore, not sensitive to any parameter, we exclude the first term in the definition of force functions $f_\alpha$ and $f_\beta$.

### 5.1.2. Model Error: type-II.

In model error type-II, we consider the input of model to be fixed, i.e., $u = u^*$, however, changing parameters makes the fractional model to result in the varied output $f^q$ as opposed to $f^*$. Therefore, we define the model error as the difference between varied and exact outputs, i.e., $E(q) = \| f^q - f^* \|_{L^2}$. The schematic of variation of model from the exact model is shown in Fig. 3 (b). In this case, unlike model error type-I, the model error and its gradient can be expressed analytically. Therefore, they do not contain any discretization error.

### 5.2. Model Error Minimization: Iterative Algorithm.

We minimize the model error by formulating a two-stages algorithm. Since we do not have prior information about the varied solution/force function, it is difficult to analytically predict the behavior of introduced model error. However, in every example, we numerically study the behavior of a low resolution model error manifold on a coarse grid, and then, perform the local minimization.

The minimization problem is written as:

$$
\min_{q \in Q} (E(q)),
$$

in which $E(q) : Q \rightarrow \mathbb{R}$, and we assume that the problem is solvable, i.e., there exist a minimum point $q^* \in Q$. Proper choice of initial guess in local minimization is of great importance, where a wrong initial guess, not falling within small enough adjacency of minimum, may never converge. Therefore, the iterative convergence in a hypercube space of parameters is highly connected to an optimal initial guess for each parameter. In the sequel, we delineate the two stages of our algorithm, namely, stage I: coarse grid searching, and stage II: nearby solution.

In stage I, we progressively divide the hypercube parameter space into subspaces to narrow down the objective search region into a smaller region. This division process is not necessarily unique and can be done in different ways, among which we discuss the easy-to-implement one here, where in each progression step, we choose the subspace with minimum error at its corner. We carry out the coarse grid searching till we reach a small enough region, in which the nearby solution (stage II) is valid. As an example, we consider a $(1+1)$-D fractional model with $q^* = \{\alpha^*, \beta^*\} = \{0.3, 0.8\}$ as the exact fractional indices in the parameter surface, shown in Fig. 4. We divide the parameter space into four equal subspaces and by computing the error at corner points of each subsurface (black dots), we shrink the search region (to the labeled subsurface 3). We progress further once again in a similar fashion, divide the subsurface, and compute the error at corner points (red dots). We finally, narrow down the search region into labeled subsurface 31. We see that in this case, with computing the error only at 14 points, we can efficiently narrow down the parameter space into a small enough search region, in which we can perform stage II of the algorithm.

In stage II of the algorithm, we employ a gradient decent method, in which by starting from an initial guess $q^0 = \{\alpha_0^0, \beta_0^0, \beta_2^0, \cdots, \beta_d^0\}$ in the obtained search region from stage I, we produce a minimizing sequence $q^i, i = 1, 2, \cdots$, where

$$
q^{i+1} = q^i + \Delta q^i,
$$

and the increment $\Delta q^i = s^i p^i$ contains both the step size $s^i$ and normalized step direction $p^i$. The superscript $i$ indicates the iteration index. We obtain the normalized direction $p^i$ by computing the gradient of model error with respect to the parameters. The step size is usually
computed by performing a line search such that $E(q^i + s p^i)$ is minimized over $\forall s \in \mathbb{R}$. However, in our case the method does not produce well-scaled search directions, and we need to approximate the current step size, using the previous one. Thus,

$$p^i = -\frac{\nabla E(q^i)}{\|\nabla E(q^i)\|}, \quad s^i = s^{i-1} \frac{\nabla E(q^{i-1})^T p^{i-1}}{\nabla E(q^i)^T p^i},$$

where the first iteration size is obtained, using the Taylor expansion of model error about $q^0$.

### 5.3. Fractional Model Construction: FSEM-based Iterative Algorithm

Let $\Omega = [0, T] \times [-1, 1]$ be the computational domain. We consider the $(1 + 1)$-D case of FPDE (3.1), subject to the initial and boundary conditions (3.2) and (3.3), respectively, where the adjoint FSEs are given in (4.11). Assuming that the exact transport field $u^*(t, x)$ and force function $f^*(t, x)$ are given, then,

$$\partial_t^\alpha u^* - k (\partial_x^\beta u^* + \partial_x^\beta u^*) = f^*$$

in which $\{\alpha^*, \beta^*\}$ are the exact fractional indices and the coefficient $k$ is known.

By considering the two types of model error, we use the developed iterative formulation and follow Algorithm 1 and Algorithm 2 to obtain the optimal model parameters. In each iteration, the increments are obtained, using (5.4).

**Remark 5.1.** In the first iteration, we compute the step size, using the Taylor expansion of the model error about the initial guess $\{\alpha^0, \beta^0\}$, which we separate into two directions as

$$E\big|_{[\alpha^0, \beta^0]} \approx E\big|_{[\alpha^0, \beta^0]} + S_{E, \alpha}\big|_{[\alpha^0, \beta^0]} (\alpha^* - \alpha^0), \quad E\big|_{[\alpha^0, \beta^0]} \approx E\big|_{[\alpha^0, \beta^0]} + S_{E, \beta}\big|_{[\alpha^0, \beta^0]} (\beta^* - \beta^0).$$

Knowing that $E\big|_{[\alpha^0, \beta^0]} = 0$, we obtain the parameters at next iterations as $\alpha^1 = \alpha^0 + \Delta \alpha^0$ and $\beta^1 = \beta^0 + \Delta \beta^0$, in which

$$\Delta \alpha^0 \approx -\frac{E\big|_{[\alpha^0, \beta^0]}}{S_{E, \alpha}\big|_{[\alpha^0, \beta^0]}}, \quad \Delta \beta^0 \approx -\frac{E\big|_{[\alpha^0, \beta^0]}}{S_{E, \beta}\big|_{[\alpha^0, \beta^0]}}.$$
Algorithm 1 Fractional Model Construction: FSEM based Iterative Algorithm (Model Error type-I)

1: Initial guess \( q^0 = (\alpha^0, \beta^0) \)
2: Do \( i = 0, 1, \cdots \)
3: Solve for \( u_N^i \): FPDE
4: Compute the model error \( E = ||u_N^i - u^*||_{L^2} \)
5: \( \text{If } E < \text{tolerance, Then } \text{Break, Otherwise } \text{Continue} \)
6: Solve for sensitivity fields: FSEs
7: Compute the model error gradient using sensitivity field
8: Compute the iteration increment \( \Delta q^i \)
9: March in parameter space \( q^{i+1} = q^i + \Delta q^i \)
10: \text{End}

Algorithm 2 Fractional Model Construction: FSEM based Iterative Algorithm (Model Error type-II)

1: Initial guess \( q^0 = (\alpha^0, \beta^0) \)
2: Do \( i = 0, 1, \cdots \)
3: Compute the model error \( E = ||L^i u^* - L^i u^*||_{L^2} \)
4: \( \text{If } E < \text{tolerance, Then } \text{Break, Otherwise } \text{Continue} \)
5: Compute the model error gradient using sensitivity field (analytically available)
6: Compute the iteration increment \( \Delta q^i \)
7: March in parameter space \( q^{i+1} = q^i + \Delta q^i \)
8: \text{End}

6. Numerical Results. In the first part of numerical results, we investigate the performance of developed PG scheme in solving FPDE and the adjoint FSEs. We consider the coupled \((1+1)d\) FPDE and FSEs with one-sided fractional derivative and \( k = 1 \), as

\[
\begin{align*}
(6.1) & \quad 0 D_t^\alpha u - \beta D_x^\beta u = f, \\
(6.2) & \quad 0 D_t^\alpha S_{u,\alpha} - \beta D_x^\beta S_{u,\alpha} = S_{f,\alpha} - A_1(\alpha) 0 D_t^\alpha u + L_1^\alpha D_t^\alpha u, \\
(6.3) & \quad 0 D_t^\alpha S_{u,\beta} - \beta D_x^\beta S_{u,\beta} = S_{f,\beta} + A_2(\beta) -1 D_t^\alpha u - L_2^\beta D_t^\beta u.
\end{align*}
\]

We consider two cases of exact solution as
- Case I: \( u^{ext}(t, x) = t^{3+\alpha/2} \left( (1 + x)^{1+\beta/2} - \frac{1}{\beta}(1 + x)^{4+\beta/2} \right) \)
- Case II: \( u^{ext}(t, x) = t^{3+\alpha/2}(t - 0.4)(t - 0.9) \left((1 + x)^{3+\beta/2} - \frac{1}{\beta}(1 + x)^{4+\beta/2}\right) \)

where \( \alpha/2 = 0.25 \), and \( \beta/2 = 0.75 \). The exact solution and sensitivity fields, obtained by taking \( \frac{\partial}{\partial x} \) and \( \frac{\partial}{\partial \beta} \) of the exact solutions, are shown in Fig. 5 and 6 for the two cases I and II, respectively. We employ the developed PG method to solve FPDE (6.1) and obtain \( u_N \), which we use to construct the right hand side of adjoint FSEs. Then, we again employ the developed PG method to solve FSEs (6.2) and (6.3) and obtain the numerical sensitivity fields, \( S_{N,\alpha} \), \( S_{N,\beta} \). We study the \( L^2 \)-norm convergence of our proposed method by increasing the number of basis functions, as shown in Fig. 7.

- Fractional Model Construction. The second part of numerical results is dedicated to study the efficiency of developed iterative algorithm in obtaining the set of model parameters \( q \) (fractional indices) and thus, construct the fractional model. We test our developed scheme by method of fabricated solution, assuming a given set of input (exact solution) and output (force term) for our fractional model.
We begin with a fractional IVP of the form \( \alpha D_t^\alpha u(t) = f(t) \), \( \alpha \in (0, 1) \), and assume that the exact solution and force function are given as,

\[
\begin{align*}
  u^*(t) &= \sin(5\pi \alpha^*/2) t^{3+\alpha^*/2}, \\
  f^*(t) &= \sin(5\pi \alpha^*/2) \frac{\Gamma(4+\alpha^*/2)}{\Gamma(4-\alpha^*/2)} t^{3-\alpha^*/2},
\end{align*}
\]

and the fractional order \( \alpha \) is the unknown model parameter. We start from an initial guess \( \alpha^0 \) and use the developed iterative algorithm to converge to the true value of fractional index \( \alpha \).

We also consider a fractional BVP of the form \( -D_x^\beta u(x) = f(x) \), \( \beta \in (1, 2) \), and assume that the exact solution and force function are given as,

\[
\begin{align*}
  u^*(x) &= (1 + x)^{3+\beta^*/2} - \frac{1}{2} (1 + x)^{3+\beta^*/2} \\
  f^*(x) &= \frac{\Gamma(4+\beta^*/2)}{\Gamma(4-\beta^*/2)} (1 + x)^{3-\beta^*/2} - \frac{1}{2} \frac{\Gamma(5+\beta^*/2)}{\Gamma(5-\beta^*/2)} (1 + x)^{2+\beta^*/2},
\end{align*}
\]

and the fractional order \( \beta \) is the unknown model parameter. We again use the developed iterative algorithm to capture the true value of fractional index \( \beta \), starting from an initial guess \( \beta^0 \).

Tables 1 and 2 show two examples for each case of fractional IVP and BVP, where the true values of fractional orders are \( \alpha^* = 0.3 \), \( \alpha^* = 0.9 \), \( \beta^* = 1.1 \), and \( \beta^* = 1.7 \). We observe that the proposed iterative formulation converges accurately to the exact values with in few numbers of iterations. We note that in the case of fractional IVP and BVP, the search region is already small enough so that the nearby solution is valid, and therefore, we only need to perform the second stage of iterative algorithm.
Fig. 7: PG spectral method, $L^2$-norm convergence study: $(1+1)$-d FPDE adjoint to corresponding FSEs with one-sided fractional derivative, $k = 1$, $\alpha/2 = 0.25$, and $\beta/2 = 0.75$, for Case I (left) and Case II (right), where $N = M$.

Table 1: Fractional model construction for the two cases of fractional IVP.

| Iteration Index | $\alpha'$ | $\alpha''$ |
|-----------------|------------|------------|
| initial guess   | 0.300000   | 0.900000   |
| 1               | 0.971980   | 0.320520   |
| 2               | 0.900418   | 0.300068   |
| 3               | 0.900000   | 0.300000   |
| True Value      | 0.9        | 0.3        |

Moreover, we consider FPDE of the form $\alpha_0 D_{\alpha}^\alpha u - k \alpha_1 D_{\beta}^\beta u = f$. We assume the exact solution $u^* = t^{1+\alpha'/2}(1+x)^{\alpha''/2} - \frac{1}{2}(1+x)^{\alpha''/2}$ and plug it into the FPDE with given $\{\alpha^*, \beta^*\}$ to obtain the exact force function $f^*$. We study the example, in which, $\{\alpha^*, \beta^*\} = \{0.1, 1.64\}$. We perform the two stages of iterative algorithm, where in the first stage, we shrink down the search region 16 time smaller than the original size, by computing the model error at 8 points (See Fig. 8, right). Then, in the next stage, we start from the initial guess $\{\alpha^0, \beta^0\} = \{0.125, 1.75\}$, and observe that the developed iterative method converges to a close neighborhood of true values $\{0.1, 1.64\}$ within $10^{-7}$ tolerance.

The developed model construction method can also be applied in formulating fractional models to study complex time-varying nonlinear fluid-solid interaction phenomena [5, 3, 2] and also the effect of damping in structural vibrations [65, 1].

7. Summary. We developed a fractional sensitivity equation method (FSEM) in order to analyze the sensitivity of fractional models (FIVPs, FBVPs, and FPDEs) with respect to their parameters. We derived the adjoint governing dynamics of sensitivity coefficients, i.e. fractional sensitivity equations (FSEs), by taking the partial derivative of FDE with respect to the model parameters, and showed that they preserve the structure of original FDE. We also introduced a new fractional operator, associated with logarithmic-power law kernel, for the first time in the context of FSEM. We extended the existing proper underlying function spaces to respect the extra regularities imposed by FSEs and proved the well-posedness of problem. Moreover, we developed a Petrov-Galerkin (PG) spectral method by employing Jacobi polyfractonomials and Legendre polynomials as basis/test functions, and proved its stability. We further used the developed FSEM to formulate an optimization problem in order
Table 2: Fractional model construction for the two cases of fractional BVP.

| Iteration Index | $\beta_1$ | $\beta_2$ |
|-----------------|-----------|-----------|
| initial guess   | 1.100000  | 1.900000  |
| 1               | 1.882020  | 1.228040  |
| 2               | 1.708120  | 1.106096  |
| 3               | 1.700020  | 1.100016  |
| 4               | 1.700000  | 1.100000  |

| True Value      | 1.7       | 1.1       |

Fig. 8: Fractional model construction for the case FPDE, using FSEM based iterative algorithm. The true values of fractional indices are $\{\alpha^*, \beta^*\} = \{0.1, 1.64\}$.

to construct the fractional model by estimating the model parameters. We defined two types of model error as objective functions and proposed a two-stages search algorithm to minimize them. We presented the steps of iterative algorithm in a pseudo code. Finally, we examined the performance of proposed numerical scheme in solving coupled FPDE and FSEs, where we numerically study the convergence rate of error. We also investigated the efficiency of developed iterative algorithm in estimating the derivative order for different cases of fractional models.
Appendix A. Proof of Lemma (2.2).

Part A: $\sigma \in (0, 1)$. We start from the $RL - PL$ definition, given in (2.8).

(A.1)

\[ RL_{a}^{LP} D_{x}^{\sigma} u = \frac{1}{\Gamma(1 - \sigma)} \frac{d}{dx} \int_{a}^{x} (x - s)^{-\sigma} \log(x - s) u(s) \, ds, \quad \text{(integrate by parts)} \]

\[ = \frac{1}{\Gamma(1 - \sigma)} \frac{d}{dx} \left[ u(s)(x - s)^{1-\sigma} \right]_{s=a}^{s=x} \]

\[ - \int_{a}^{x} \frac{d}{ds} \left[ (x - s)^{-\sigma + 1} \right] (1 - (-\sigma + 1) \log(x - s)) \, ds, \]

\[ = \frac{1}{\Gamma(1 - \sigma)} \frac{d}{dx} \left[ u(a)(x - a)^{1-\sigma} \right] (1 - (-\sigma + 1) \log(x - a)) \]

\[ - \int_{a}^{x} \frac{d}{ds} \left[ (x - s)^{-\sigma + 1} \right] (1 - (-\sigma + 1) \log(x - s)) \, ds, \]

\[ = \frac{u(a)}{\Gamma(1 - \sigma)} \frac{\log(x - a)}{(x - a)^{\sigma}} + \frac{1}{\Gamma(1 - \sigma)} \int_{a}^{x} \frac{\log(x - s)}{(x - s)^{-\sigma}} u'(s) \, ds, \quad \text{(by Leibnitz rule)} \]

\[ = \frac{u(a)}{\Gamma(1 - \sigma)} \frac{\log(x - a)}{(x - a)^{\sigma}} + c_{-LP}^{\alpha} D_{x}^{\alpha} u. \]

Part B: $\sigma \in (1, 2)$. Similarly, we start from the $RL - PL$ definition, given in (2.8).

(A.2)

\[ RL_{a}^{LP} D_{x}^{\sigma} u = \frac{1}{\Gamma(2 - \sigma)} \frac{d^2}{dx^2} \int_{a}^{x} (x - s)^{-\sigma + 1} \log(x - s) u(s) \, ds, \quad \text{(integrate by parts twice)} \]

\[ = \frac{1}{\Gamma(2 - \sigma)} \frac{d^2}{dx^2} \left[ u(s)(x - s)^{-\sigma + 2} \right]_{s=a}^{s=x} \]

\[ - \frac{u'(s)(x - s)^{-\sigma + 3}}{(-\sigma + 2)(-\sigma + 3)^2} (1 - 2(-\sigma + 3) + (-\sigma + 3)(-\sigma + 2) \log(x - s)) \bigg|_{s=a}^{s=x} \]

\[ + \int_{a}^{x} \frac{(x - s)^{-\sigma + 3}}{(-\sigma + 2)(-\sigma + 3)^2} \left( 1 - 2(-\sigma + 3) + (-\sigma + 3)(-\sigma + 2) \log(x - s) \right) u''(s) \, ds, \]

\[ = \frac{1}{\Gamma(2 - \sigma)} \frac{d^2}{dx^2} \left[ u(a)(x - a)^{-\sigma + 2} \right]_{s=a}^{s=x} \]

\[ - \frac{u'(a)(x - a)^{-\sigma + 3}}{(-\sigma + 2)(-\sigma + 3)^2} (1 - 2(-\sigma + 3) + (-\sigma + 3)(-\sigma + 2) \log(x - a)) \bigg|_{s=a}^{s=x} \]

\[ + \int_{a}^{x} \frac{(x - s)^{-\sigma + 3}}{(-\sigma + 2)(-\sigma + 3)^2} \left( 1 - 2(-\sigma + 3) + (-\sigma + 3)(-\sigma + 2) \log(x - s) \right) u''(s) \, ds, \]

\[ = \frac{u(a)}{\Gamma(2 - \sigma)} \frac{1 + (\sigma + 1) \log(x - a)}{(x - a)^{\sigma}} + \frac{u'(a)}{\Gamma(2 - \sigma)} \frac{\log(x - a)}{(x - a)^{\sigma - 1}} \]

\[ + \frac{1}{\Gamma(2 - \sigma)} \int_{a}^{x} (x - s)^{-\sigma + 1} \log(x - s) u''(s) \, ds, \quad \text{(by Leibnitz rule)} \]

\[ = \frac{u(a)}{\Gamma(1 - \sigma)} \frac{1 + (\sigma + 1) \log(x - a)}{(x - a)^{\sigma}} + \frac{u'(a)}{\Gamma(1 - \sigma)} \frac{\log(x - a)}{(x - a)^{\sigma - 1}} + c_{-LP}^{\alpha} D_{x}^{\alpha} u. \]

Appendix B. Proof of Lemma (2.3).

In Lemma 2.1 in [33] and also in [19], it is shown that $\| \cdot \|_{H^{\alpha}(\Lambda)}$ and $\| \cdot \|_{H^{\alpha}(\Lambda)}$ are
equivalent. Therefore, for \( u \in H^r(\Lambda) \), there exist positive constants \( C_1 \) and \( C_2 \) such that

\[
\|u\|_{H^r(\Lambda)} \leq C_1 \|u\|_{H^r(\Lambda)}, \quad \|u\|_{H^r(\Lambda)} \leq C_2 \|u\|_{H^r(\Lambda)},
\]

which leads to

\[
\|u\|^2_{H^r(\Lambda)} \leq C_1^2 \|u\|^2_{H^r(\Lambda)} + C_2^2 \|u\|^2_{H^r(\Lambda)},
\]

\[
= C_1^2 \|a \mathcal{D}_x^r (u)\|^2_{L^2(\Lambda)} + C_2^2 \|s \mathcal{D}_y^r (u)\|^2_{L^2(\Lambda)} + (C_1^2 + C_2^2) \|u\|^2_{L^2(\Lambda)},
\]

\[
\leq \tilde{C}_1 \|u\|^2_{H^r(\Lambda)},
\]

where \( \tilde{C}_1 \) is a positive constant. Similarly, we can show that \( \|u\|^2_{H^r(\Lambda)} \leq \tilde{C}_2 \|u\|^2_{H^r(\Lambda)} \), where \( \tilde{C}_2 \) is a positive constant.

**Appendix C. Proof of Lemma (2.5).** \( X_1 \) is endowed with the norm \( \| \cdot \|_{X_1} \), where \( \| \cdot \|_{X_1} \equiv \| \cdot \|_{H^{1/2}(\Lambda)} \) by Lemma 2.3. Moreover, \( X_2 \) is associated with the norm

\[
\| \cdot \|_{X_2} = \left\{ \| \cdot \|^2_{H^{1/2}(\Lambda)} + \| \cdot \|^2_{L^2(\Lambda)} \right\}^{1/2},
\]

where

\[
\|u\|^2_{H^{1/2}(\Lambda)} = \int_{\Lambda^2} \left( \int_{\Lambda^2} |a \mathcal{D}_x^{1/2} u|^2 d\tau \right) dx + \int_{\Lambda^2} \left( \int_{\Lambda^2} |s \mathcal{D}_y^{1/2} u|^2 d\tau \right) dx + \int_{\Lambda} |u|^2 d\tau
\]

\[
= \int_{\Lambda} \left( \int_{\Lambda} |a \mathcal{D}_x^{1/2} u|^2 d\tau \right) dx + \int_{\Lambda} \left( \int_{\Lambda} |s \mathcal{D}_y^{1/2} u|^2 d\tau \right) dx + \int_{\Lambda} |u|^2 d\tau
\]

\[
= \|a \mathcal{D}_x^{1/2} (u)\|^2_{L^2(\Lambda)} + \|s \mathcal{D}_y^{1/2} (u)\|^2_{L^2(\Lambda)} + \|u\|^2_{L^2(\Lambda)},
\]

and

\[
\|u\|^2_{L^2(\Lambda)} = \int_{\Lambda} \left( \int_{\Lambda} |a \mathcal{D}_x^{1/2} u|^2 d\tau \right) dx + \int_{\Lambda} \left( \int_{\Lambda} |s \mathcal{D}_y^{1/2} u|^2 d\tau \right) dx + \int_{\Lambda} |u|^2 d\tau
\]

\[
= \|a \mathcal{D}_x^{1/2} u\|^2_{L^2(\Lambda)} + \|s \mathcal{D}_y^{1/2} u\|^2_{L^2(\Lambda)} + \|u\|^2_{L^2(\Lambda)}.
\]

We use the mathematical induction to carry out the proof. Therefore, we assume the following equality holds

\[
\| \cdot \|_{X_k} \equiv \left\{ \sum_{i=1}^{k-1} \| \mathcal{D}_x^{1/2} (\cdot)\|^2_{L^2(\Lambda_{i,k-1})} + \| a \mathcal{D}_x^{1/2} (\cdot)\|^2_{L^2(\Lambda_{i,k-1})} + \| \cdot \|^2_{L^2(\Lambda_{i,k-1})} \right\}^{1/2}.
\]
Since,
\[
\|u\|_{L^2((a_i, b_i); L^2(\Lambda_{k-1}))}^2 \\
= \int_{\Lambda_{k-1}} \left( \int_{a_i}^{b_i} |a_i \mathcal{D}_{x_k}^{\hat{h}/2} u|_2^2 \, dx_k + \int_{a_i}^{b_i} |x_k \mathcal{D}_{x_k}^{\hat{h}/2} u|_2^2 \, dx_k + \int_{a_i}^{b_i} |u|_2^2 \, dx_k \right) \, d\Lambda_{k-1} \\
= \int_{\Lambda_{k-1}} \int_{a_i}^{b_i} |a_i \mathcal{D}_{x_k}^{\hat{h}/2} u|_2^2 \, dx_k \, d\Lambda_{k-1} + \int_{\Lambda_{k-1}} \int_{a_i}^{b_i} |x_k \mathcal{D}_{x_k}^{\hat{h}/2} u|_2^2 \, dx_k \, d\Lambda_{k-1} + \int_{\Lambda_{k-1}} \int_{a_i}^{b_i} |u|_2^2 \, dx_k \, d\Lambda_{k-1} \\
= \| a_i \mathcal{D}_{x_k}^{\hat{h}/2} (u) \|_{L^2(\Lambda_k)}^2 + \| x_k \mathcal{D}_{x_k}^{\hat{h}/2} (u) \|_{L^2(\Lambda_k)}^2 + \| u \|_{L^2(\Lambda_k)}^2,
\]
and
\[
\|u\|_{L^2((a_i, b_i); L^2(\Lambda_{k-1}))}^2 = \int_{a_i}^{b_i} \left( \int_{\Lambda_{k-1}} \int_{a_i}^{b_i} |a_i \mathcal{D}_{x_k}^{\hat{h}/2} u|_2^2 \, dx_k \, d\Lambda_{k-1} + \int_{\Lambda_{k-1}} \int_{a_i}^{b_i} |x_k \mathcal{D}_{x_k}^{\hat{h}/2} u|_2^2 \, dx_k \, d\Lambda_{k-1} + \int_{\Lambda_{k-1}} \int_{a_i}^{b_i} |u|_2^2 \, dx_k \, d\Lambda_{k-1} \right) \, dx_k \\
= \int_{a_i}^{b_i} \left( \int_{\Lambda_{k-1}} \int_{a_i}^{b_i} |a_i \mathcal{D}_{x_k}^{\hat{h}/2} u|_2^2 \, dx_k \, d\Lambda_{k-1} + \int_{\Lambda_{k-1}} \int_{a_i}^{b_i} |x_k \mathcal{D}_{x_k}^{\hat{h}/2} u|_2^2 \, dx_k \, d\Lambda_{k-1} + \int_{\Lambda_{k-1}} \int_{a_i}^{b_i} |u|_2^2 \, dx_k \, d\Lambda_{k-1} \right) \, dx_k \\
= \sum_{i=1}^{k-1} \left( \int_{\Lambda_i} \int_{a_i}^{b_i} |a_i \mathcal{D}_{x_k}^{\hat{h}/2} u|_2^2 \, dx_k \, d\Lambda_{k-1} + \int_{\Lambda_i} \int_{a_i}^{b_i} |x_k \mathcal{D}_{x_k}^{\hat{h}/2} u|_2^2 \, dx_k \, d\Lambda_{k-1} + \int_{\Lambda_i} \int_{a_i}^{b_i} |u|_2^2 \, dx_k \, d\Lambda_{k-1} \right),
\]
we can show that
\[
\text{(C.5)} \quad \| \cdot \|_{\mathcal{X}_i} \equiv \left\{ \sum_{i=1}^{k} \left( \| a_i \mathcal{D}_{x_k}^{\hat{h}/2} (\cdot) \|_{L^2(\Lambda_i)}^2 + \| x_i \mathcal{D}_{x_k}^{\hat{h}/2} (\cdot) \|_{L^2(\Lambda_i)}^2 + \| \cdot \|_{L^2(\Lambda_i)}^2 \right) \right\}^{\frac{1}{2}}.
\]

**Appendix D. Proof of Lemma (2.8).** According to [30], we have
\[
(a_i \mathcal{D}_{x_k}^{\hat{h}/2} u, v)_{\Lambda_i} = \int_{\Lambda_i} \frac{1}{(1-\beta/2)} \left[ \frac{d}{dx_i} \int_{x_i}^{x_i} \frac{\bar{u}(s) \, ds}{(x_i - s_i)^{\hat{h}/2}} \right] v \, d\Lambda_d
\]
\[
= \left[ (1-\beta/2) x_i^{\hat{h}/2} \right]_{x_i=a_i}^{b_i} \int_{\Lambda_i} \frac{1}{(1-\beta/2)} \left[ \frac{d}{dx_i} \right] \left[ \frac{\bar{u}(s) \, ds}{(x_i - s)^{\hat{h}/2}} \right] v \, d\Lambda_d.
\]
Based on the homogeneous boundary conditions, \( \left[ (1-\beta/2) x_i^{\hat{h}/2} \right]_{x_i=a_i}^{b_i} = 0 \). Therefore,
\[
(a_i \mathcal{D}_{x_k}^{\hat{h}/2} u, v)_{\Lambda_i} = - \int_{\Lambda_i} \frac{1}{(1-\beta/2)} \left[ \frac{d}{dx_i} \right] \left[ \frac{\bar{u}(s) \, ds}{(x_i - s)^{\hat{h}/2}} \right] v \, d\Lambda_d.
\]
Moreover, we find that
\[
\frac{d}{ds} \int_{x_i}^{b_i} \frac{u}{(x_i - s)^{\hat{h}/2}} \, dx_i = \frac{d}{ds} \left[ \frac{v(x_i - s)^{1-\hat{h}/2}}{1-\beta/2} \right]_{x_i=x_i}^{x_i=x_i} - \frac{1}{1-\beta/2} \int_{x_i}^{b_i} \frac{dv}{dx_i} (x_i - s)^{1-\hat{h}/2} \, dx_i
\]
\[
= -\frac{1}{1-\beta/2} \int_{x_i}^{b_i} \frac{dv}{dx_i} (x_i - s)^{1-\hat{h}/2} \, dx_i = \int_{x_i}^{b_i} \frac{dv}{dx_i} (x_i - s)^{1-\hat{h}/2} \, dx_i.
\]
Therefore, we get
\[
(a_i \mathcal{D}_{x_k}^{\hat{h}/2} u, v)_{\Lambda_i} = - \int_{\Lambda_i} \frac{1}{(1-v)} \bar{u}(s) - \frac{d}{ds} \int_{x_i}^{b_i} \frac{v}{(x_i - s)^{\hat{h}/2}} \, dx_i \, ds = (\bar{u}, x_i \mathcal{D}_{x_k}^{\hat{h}/2} v)_{\Lambda_i}.
\]
Appendix E. Proof of Lemma (4.4). We know that

\[ \left| \left( D_t^{\eta/2} u, D_T^{\eta/2} v \right)_\Omega \right| = \left( \int_{\Lambda_d} \int_0^T \left| D_t^{\eta/2} u \cdot D_T^{\eta/2} v \right|^2 \, dt \, d \Lambda_d \right)^{\frac{1}{2}}. \]

Therefore, by Hölder inequality

\[ \left| \left( D_t^{\eta/2} u, D_T^{\eta/2} v \right)_\Omega \right| \leq \left( \int_{\Lambda_d} \int_0^T \left| D_t^{\eta/2} u \right|^2 \, dt \, d \Lambda_d \right)^{\frac{1}{2}} \left( \int_{\Lambda_d} \int_0^T \left| D_T^{\eta/2} v \right|^2 \, dt \, d \Lambda_d \right)^{\frac{1}{2}} \]

\[ \leq \left( \int_{\Lambda_d} \int_0^T \left| D_t^{\eta/2} u \right|^2 \, dt \, d \Lambda_d + \int_{\Lambda_d} \int_0^T \left| u \right|^2 \, dt \, d \Lambda_d + \int_0^T \left| v \right|^2 \, dt \, d \Lambda_d \right)^{\frac{1}{2}} \]

\[ = \| D_t^{\eta/2} u \|_{L^2(\Omega)} \| D_T^{\eta/2} v \|_{L^2(\Omega)} = \| u \|_{H^{\eta/2}(\Omega)} \| v \|_{H^{\eta/2}(\Omega)}. \]

Moreover, by equivalence of \( | \cdot |_{H^{\eta/2}} = | \cdot |_{H^{\eta/2}} \) and \( | \cdot |_{H^{\eta/2}} \), we have

\[ \left( D_t^{\eta/2} u, D_T^{\eta/2} v \right)_I = \int_0^T \left| D_t^{\eta/2} u \right|^2 \, dt \]

\[ \geq \int_{\Lambda_d} \int_0^T \left| D_t^{\eta/2} u \right|^2 \, dt \left( \int_{\Lambda_d} \int_0^T \left| D_T^{\eta/2} v \right|^2 \, dt \right) \]

\[ \geq \beta \int_{\Lambda_d} \int_0^T \left| D_t^{\eta/2} u \right|^2 \, dt \, d \Lambda_d \int_0^T \left| D_T^{\eta/2} v \right|^2 \, dt \, d \Lambda_d \]

\[ \geq \beta \| u \|_{H^{\eta/2}(\Omega)} \| v \|_{H^{\eta/2}(\Omega)}, \]

where \( 0 < \beta_1 \leq 1 \).

Appendix F. Proof of The Stability Theorem (4.6).

Part A: \( d = 1 \). It is evident that \( u \) and \( v \) are in Hilbert spaces (see [19, 33]). For \( 0 < \beta \leq 1 \), we have

\[ |a(u, v)| = |\left( D_t^{\eta/2} (u), D_T^{\eta/2} (v) \right)_\Omega + \left( a_i, D_t^{\eta/2} (u), x_i, D_T^{\eta/2} (v) \right)_\Omega + \left( a_i, D_t^{\eta/2} (u), x_i, D_T^{\eta/2} (v) \right)_\Omega| + |u, v|_\Omega| \]

\[ \geq \beta \left( |\left( D_t^{\eta/2} (u), D_T^{\eta/2} (v) \right)_\Omega| + |a_i, D_t^{\eta/2} (u), x_i, D_T^{\eta/2} (v) \right)_\Omega| + |u, v|_\Omega \right), \]

since \( \sup_{u \in D} |a(u, v)| > 0 \). Next, by equivalence of spaces and their associated norms, (4.36), and (4.37), we obtain

\[ |\left( D_t^{\eta/2} (u), D_T^{\eta/2} (v) \right)_\Omega| \geq C_1 \| D_t^{\eta/2} (u) \|_{L^2(\Omega)} \| D_T^{\eta/2} (v) \|_{L^2(\Omega)}, \]

\[ |a_i, D_t^{\eta/2} (u), x_i, D_T^{\eta/2} (v) \right)_\Omega| \geq C_2 \| a_i, D_t^{\eta/2} (u) \|_{L^2(\Omega)} \| D_T^{\eta/2} (v) \|_{L^2(\Omega)}, \]
and
\[ |(x, D_{y_1}^{\alpha/2} u, a, D_{y_2}^{\alpha/2} v)_{\Omega}| \geq C_3 \| x \| D_{y_1}^{\alpha/2} u \|_{L^2} \| a \| D_{y_2}^{\alpha/2} v \|_{L^2}, \]
where \( C_1, C_2, \) and \( C_3 \) are positive constants. Therefore,
\[ |a(u, v)| \geq C\beta \| x \| D_{y_1}^{\alpha/2} u \|_{L^2} \| a \| D_{y_2}^{\alpha/2} v \|_{L^2} + \| a \| D_{y_1}^{\alpha/2} u \|_{L^2} \| x \| D_{y_2}^{\alpha/2} v \|_{L^2}, \]
where \( C \) is \( \min\{C_1, C_2, C_3\}. \) Also, the norm \( \| x \|_{L^2} \| a \|_{L^2} \) is equivalent to the right hand side of inequality (F.2). Therefore, \( |a(u, v)| \geq C \| x \|_{L^2} \| a \|_{L^2}. \)

**Part B:** \( d > 1. \) Similarly, we have
\[ |a(u, v)| \geq \beta \left( |(0, D_{x_1}^{\alpha/2} u, a, D_{x_2}^{\alpha/2} v)_{\Omega}| + \sum_{i=1}^{d} \left( |(x, D_{y_1}^{\alpha/2} u, a, D_{y_2}^{\alpha/2} v)_{\Omega}| + |(x, D_{y_1}^{\alpha/2} u, a, D_{y_2}^{\alpha/2} v)_{\Omega}| \right) \right), \]
where \( 0 < \beta \leq 1. \) Recalling that as the direct consequences of (4.36), we obtain
\[ |(x, D_{y_1}^{\alpha/2} u, a, D_{y_2}^{\alpha/2} v)_{\Omega}| = \| x \| D_{y_1}^{\alpha/2} u \|_{L^2} \| a \| D_{y_2}^{\alpha/2} v \|_{L^2}, \]
\[ |(x, D_{y_1}^{\alpha/2} u, a, D_{y_2}^{\alpha/2} v)_{\Omega}| = \| x \| D_{y_1}^{\alpha/2} u \|_{L^2} \| a \| D_{y_2}^{\alpha/2} v \|_{L^2}. \]
Thus,
\[ \sum_{i=1}^{d} \left( |(x, D_{y_1}^{\alpha/2} u, a, D_{y_2}^{\alpha/2} v)_{\Omega}| \right), \]
\[ \geq C \sum_{i=1}^{d} \left( \| x \| D_{y_1}^{\alpha/2} u \|_{L^2} \| a \| D_{y_2}^{\alpha/2} v \|_{L^2} \right), \]
\[ \geq \tilde{C}_1 \beta \sum_{i=1}^{d} \left( \| x \| D_{y_1}^{\alpha/2} u \|_{L^2} \| a \| D_{y_2}^{\alpha/2} v \|_{L^2} \right) \times \sum_{i=1}^{d} \left( \| x \| D_{y_2}^{\alpha/2} v \|_{L^2} \right). \]
for \( u, v \in L^2(I; X), \) where \( 0 < \tilde{C} \) and \( 0 < \tilde{\beta} \leq 1. \) Furthermore, Lemma 4.4 yields
\[ |(0, D_{x_1}^{\alpha/2} u, a, D_{x_2}^{\alpha/2} v)_{\Omega}| = \| x \|_{H^{\alpha/2}(L^2(\Omega))} \| a \|_{H^{\alpha/2}(L^2(\Omega))}, \]
Therefore, from (F.4) and (F.5) we have
\[ |a(u, v)| \geq \beta \left( \| x \|_{H^{\alpha/2}(L^2(\Omega))} \| a \|_{H^{\alpha/2}(L^2(\Omega))} + \| u \|_{L^2(I; X)} \| v \|_{L^2(I; X)} \right), \]
where
\[ \| u \|_{H^{\alpha/2}(L^2(\Omega))} \| v \|_{H^{\alpha/2}(L^2(\Omega))} + \| u \|_{L^2(I; X)} \| v \|_{L^2(I; X)}, \]
\[ \geq C_2 \left( \| u \|_{H^{\alpha/2}(L^2(\Omega))} + \| u \|_{L^2(I; X)} \right) \left( \| v \|_{H^{\alpha/2}(L^2(\Omega))} + \| v \|_{L^2(I; X)} \right) \]
for \( u \in U, v \in U \) and \( 0 < C_2 \leq 1. \) By considering (F.6) and (F.7), we get
\[ |a(u, v)| \geq C \| x \|_{L^2} \| a \|_{L^2}. \]
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