Boundary Conditions for Two-Sided (and Tempered) Fractional Diffusion

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Motivation

- Two-sided fractional diffusion equations are important in many applications: transport in heterogeneous porous media (Benson et al., 2000), turbulence modeling (Chen, 2006), (del-Castillo Negrete et al., 2004), (Gunzburger et al., 2018), and biomedical acoustics (Treeby and Cox, 2010).
- Most numerical methods assume Dirichlet boundary conditions (BCs): (Meerschaert and Tadjeran, 2006) , (Mao and Karniadakis, 2018), (Samiee et al., 2018).
- For anomalous diffusion, a homogeneous Dirichlet BC models an *absorbing* boundary.

Motivation

- However, many of these applications involve a conserved quantity in a bounded domain.
- From a stochastic point of view, particles are *reflected* at the boundary and the total mass does not change.
- Recently, effort has been spent on developing mass-preserving, *reflecting* (Neumann) BCs for space fractional diffusion equations (Ma, 2017), (Baeumer et al., 2018a,b), (Deng et al., 2018).

One-Sided Fractional Diffusion Equation: Riemann-Liouville

- Consider one-sided space-fractional ($1 < \alpha \leq 2$) diffusion equation on $[L, R]$:

$$\frac{\partial}{\partial t} u(x,t) = C \mathbb{D}^{\alpha}_{L^+} u(x,t)$$

- The positive (left) Riemann-Liouville derivative on the bounded interval $[L, R]$ is:

$$\mathbb{D}^{\alpha}_{L^+} u(x,t) = \frac{\partial^n}{\partial x^n} I^{n-\alpha}_{L^+} u(x,t) = \frac{1}{\Gamma(n-\alpha)} \frac{\partial^n}{\partial x^n} \int_L^x \frac{u(y,t)}{(x-y)^{\alpha-n+1}} \, dy$$

- To derive *reflecting boundary conditions*, write in *conservation form*

$$\frac{\partial}{\partial t} u(x,t) + \frac{\partial}{\partial x} F_{RL}(x,t) = 0$$

with flux $F_{RL}(x,t) = -C \mathbb{D}^{\alpha-1}_{L^+} u(x,t)$.

Reflecting Boundary Conditions: Riemann-Liouville

- Assume some initial mass $M_0 = \int_L^R u(x,t)\,dx$ that is conserved for all time t.
- Integrate the mass conservation equation

$$\begin{aligned} \frac{\partial M_0}{\partial t} &= \int_L^R \frac{\partial}{\partial t} u(x,t)\,dx \\ &= -\int_L^R \frac{\partial}{\partial x} F_{RL}(x,t)\,dx \\ &= F_{RL}(L,t) - F_{RL}(R,t). \end{aligned}$$

- Imposing zero flux at the boundary $F_{RL}(L,t) = F_{RL}(R,t) = 0$ ensures mass conservation, yielding a reflecting BC (Baeumer et al., 2018a):

$$\boxed{\mathbb{D}_{L^+}^{\alpha-1} u(x,t) = 0 \text{ for } x = L \text{ and } x = R \text{ for all } t \geq 0}$$

One-Sided Fractional Diffusion Equation: Patie-Simon

- Also consider an alternative space-fractional diffusion equation

$$\frac{\partial}{\partial t} u(x,t) = C\mathbf{D}^{\alpha}_{L^+} u(x,t)$$

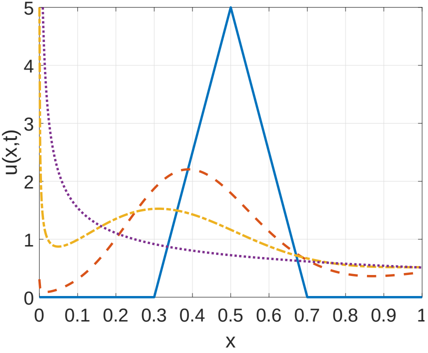
- The *Patie-Simon* (Patie and Simon, 2012) or *mixed Caputo* (Baeumer et al., 2018a) fractional derivative for $1 < \alpha \le 2$ is

$$\mathbf{D}^{\alpha}_{L^+} u(x,t) = \frac{\partial}{\partial x} \partial^{\alpha-1}_{L^+} u(x,t) = \frac{1}{\Gamma(2-\alpha)} \frac{\partial}{\partial x} \int_L^x \frac{u'(y,t)}{(x-y)^{\alpha-1}}\, dy$$

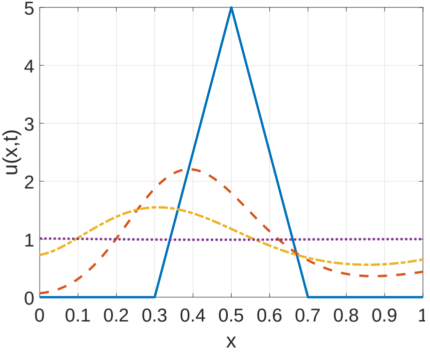
- The corresponding flux is $F_C(x,t) = -C\partial^{\alpha-1}_{L^+} u(x,t)$, where $\partial^{\alpha-1}_{L^+}$ is a Caputo derivative.
- Applying zero flux yields a reflecting BC:

$$\boxed{\partial^{\alpha-1}_{L^+} u(x,t) = 0 \text{ for } x = L \text{ and } x = R \text{ for all } t \ge 0.}$$

Numerical Solutions



(a) Riemann-Liouville flux



(b) Caputo flux

Figure: Numerical solution using a) Riemann-Liouville fractional derivative and b) Patie-Simon fractional derivative with reflecting BCs. $\alpha = 1.5$, $C = 1$ on $0 \leq x \leq 1$ at time $t = 0$ (solid line), $t = 0.05$ (dashed), $t = 0.1$ (dash dot), $t = 0.5$ (dotted).

Plan

Two-Sided Fractional Diffusion Equation: Riemann-Liouville

The *two-sided* space-fractional diffusion equation on $[L, R]$:

$$\frac{\partial}{\partial t} u(x,t) = pC\mathbb{D}^{\alpha}_{L^+} u(x,t) + qC\mathbb{D}^{\alpha}_{R^-} u(x,t) + s(x,t)$$

where $1 < \alpha \leq 2$, where $C > 0$, $p, q \geq 0$, and $p + q = 1$, while $s(x,t)$ is a source term. The *positive* (left) and *negative* (right) Riemann-Liouville fractional derivatives are given by

$$\mathbb{D}^{\alpha}_{L^+} u(x,t) = \frac{\partial^n}{\partial x^n} I^{n-\alpha}_{L^+} u(x,t) = \frac{1}{\Gamma(n-\alpha)} \frac{\partial^n}{\partial x^n} \int_L^x \frac{u(y,t)}{(x-y)^{\alpha-n+1}}\, dy$$

$$\mathbb{D}^{\alpha}_{R^-} u(x,t) = (-1)^n \frac{\partial^n}{\partial x^n} I^{n-\alpha}_{R^-} u(x,t) = \frac{(-1)^n}{\Gamma(n-\alpha)} \frac{\partial^n}{\partial x^n} \int_x^R \frac{u(y,t)}{(y-x)^{\alpha-n+1}}\, dy$$

Two-Sided Fractional Diffusion Equation: Patie-Simon

We also consider an alternative space-fractional diffusion equation

$$\frac{\partial}{\partial t}u(x,t) = pC\mathbf{D}^{\alpha}_{L^+}u(x,t) + qC\mathbf{D}^{\alpha}_{R^-}u(x,t) + s(x,t)$$

$$\mathbf{D}^{\alpha}_{L^+}u(x,t) = \frac{\partial}{\partial x}\partial^{\alpha-1}_{L^+}u(x,t) = \frac{1}{\Gamma(2-\alpha)}\frac{\partial}{\partial x}\int_L^x \frac{u'(y,t)}{(x-y)^{\alpha-1}}\,dy$$

$$\mathbf{D}^{\alpha}_{R^-}u(x,t) = -\frac{\partial}{\partial x}\partial^{\alpha-1}_{R^-}u(x,t) = \frac{1}{\Gamma(2-\alpha)}\frac{\partial}{\partial x}\int_x^R \frac{u'(y,t)}{(y-x)^{\alpha-1}}\,dy$$

using the *Patie-Simon* (Patie and Simon, 2012) or *mixed Caputo* (Baeumer et al., 2018a) fractional derivatives for $1 < \alpha \leq 2$.

$$\partial^{\alpha}_{L^+}u(x,t) = \frac{1}{\Gamma(n-\alpha)}\int_L^x \frac{u^{(n)}(y,t)}{(x-y)^{\alpha-n+1}}\,dy$$

$$\partial^{\alpha}_{R^-}u(x,t) = \frac{(-1)^n}{\Gamma(n-\alpha)}\int_x^R \frac{u^{(n)}(y,t)}{(y-x)^{\alpha-n+1}}\,dy$$

are the positive (left) and negative (right) Caputo derivatives.

Conservation Form

- Physically, $u(x,t)$ represents concentration governed by a local mass conservation (continuity) equation

$$\frac{\partial}{\partial t}u(x,t) + \frac{\partial}{\partial x}F(x,t) = 0$$

- $F(x,t)$ is a *flux function* (generalized Fick's law) that accounts for *nonlocal* diffusion.
- The flux function is given by

$$F_{RL}(x,t) = qC\mathbb{D}_{R^-}^{\alpha-1}u(x,t) - pC\mathbb{D}_{L^+}^{\alpha-1}u(x,t)$$

$$F_C(x,t) = qC\partial_{R^-}^{\alpha-1}u(x,t) - pC\partial_{L^+}^{\alpha-1}u(x,t)$$

where $F_{RL}(x,t)$ is a Riemann-Liouville flux and $F_C(x,t)$ is a Caputo flux.

Reflecting (no-flux) Boundary Conditions

- Identify a no-flux BC by setting $F(x, t) = 0$ at the boundary. Setting $F(x, t) = 0$ at $x = L$ and $x = R$ yields reflecting BCs:

$$\boxed{p\mathbb{D}_{L^+}^{\alpha-1}u(x,t) = q\mathbb{D}_{R^-}^{\alpha-1}u(x,t) \text{ for } x = L \text{ and } x = R \text{ for all } t \geq 0.}$$

$$\boxed{p\partial_{L^+}^{\alpha-1}u(x,t) = q\partial_{R^-}^{\alpha-1}u(x,t) \text{ for } x = L \text{ and } x = R \text{ for all } t \geq 0.}$$

- These boundary conditions are *nonlocal* since the BC at $x = L$ or $x = R$ depends on all values of $u(x, t)$ in the interval $[L, R]$ (if $p \neq 0$ or 1).
- If $p = 1$, these BCs reduce to the reflecting BCs proposed in (Baeumer et al., 2018a).

Other BCs

- Also consider reflecting on the left boundary and absorbing on the right boundary (reflecting/absorbing BCs)

$$\text{RL: } p\mathbb{D}_{L^+}^{\alpha-1}u(x,t) = q\mathbb{D}_{R^-}^{\alpha-1}u(x,t) \text{ for } x = L \text{ and } u(R,t) = 0$$

$$\text{C: } p\partial_{L^+}^{\alpha-1}u(x,t) = q\partial_{R^-}^{\alpha-1}u(x,t) \text{ for } x = L \text{ and } u(R,t) = 0,$$

- Absorbing on the left and reflecting on the right (absorbing/reflecting BCs)

$$\text{RL: } u(L,t) = 0 \text{ and } p\mathbb{D}_{L^+}^{\alpha-1}u(x,t) = q\mathbb{D}_{R^-}^{\alpha-1}u(x,t) \text{ for } x = R$$

$$\text{C: } u(L,t) = 0 \text{ and } p\partial_{L^+}^{\alpha-1}u(x,t) = q\partial_{R^-}^{\alpha-1}u(x,t) \text{ for } x = R.$$

- Absorbing (Dirichlet) BCs on both boundaries $u(L,t) = u(R,t) = 0$ will also be considered.

Finite-Difference Approximations

Discretize using explicit or implicit Euler scheme combined with the shifted Grünwald estimate (Meerschaert and Tadjeran, 2006)

$$\mathbb{D}^{\alpha}_{L^+} f(x_j) = h^{-\alpha} \sum_{i=0}^{j+1} g_i^{\alpha} f(x_{j-i+1}) + \mathcal{O}(h)$$

$$\mathbb{D}^{\alpha}_{R^-} f(x_j) = h^{-\alpha} \sum_{i=0}^{n-j+1} g_i^{\alpha} f(x_{j+i-1}) + \mathcal{O}(h)$$

where $h = (R - L)/n$ with Grünwald weights g_i^{α}.

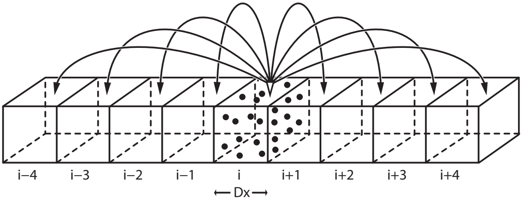


Figure: Particle interpretation of Grünwald estimate.

Finite-Difference Approximations

- The explicit Euler scheme is given by

$$u\left(x_j, t_{k+1}\right) = u\left(x_j, t_k\right) + \frac{pC\Delta t}{h^\alpha} \sum_{i=0}^{j+1} g_i^\alpha u\left(x_{j-i+1}, t_k\right)$$
$$+ \frac{qC\Delta t}{h^\alpha} \sum_{i=0}^{n-j+1} g_i^\alpha u\left(x_{j+i-1}, t_k\right) + \Delta t \; s\left(x_j, t_k\right).$$

- Define $\mathbf{u}_k = [u(x_i, t_k)]$ along with the source $\mathbf{s}_k = [\Delta t \; s(x_i, t_k)]$, yielding a matrix problem:

$$\mathbf{u}_{k+1} = \mathbf{u}_k + \beta_+ \mathbf{u}_k B^+ + \beta_- \mathbf{u}_k B^- + \mathbf{s}_k$$

where $\beta_+ = pCh^{-\alpha}\Delta t$, $\beta_- = qCh^{-\alpha}\Delta t$, and $B^\pm$ are $(n+1) \times (n+1)$ iteration matrices.

Finite-Difference Approximations

- The explicit scheme is written compactly as

$$\mathbf{u}_{k+1} = \mathbf{u}_k A + \mathbf{s}_k$$

  where $A = I + \beta_+ B^+ + \beta_- B^-$.
- Applying an implicit Euler discretization yields

$$\mathbf{u}_{k+1} = \mathbf{u}_k + \beta_+ \mathbf{u}_{k+1} B^+ + \beta_- \mathbf{u}_{k+1} B^- + \mathbf{s}_{k+1},$$

- This implicit scheme may be written as

$$\mathbf{u}_{k+1} M = \mathbf{u}_k + \mathbf{s}_{k+1},$$

  where $M = I - \beta_+ B^+ - \beta_- B^-$.

Iteration Matrix: Riemann-Liouville Flux

- Consider the Euler schemes associated with the Riemann-Liouville diffusion equation subject to reflecting BCs with B^+

$$b_{i,j} = \begin{cases} g^{\alpha}_{j-i+1} & \text{if } 0 < j < n \text{ and } i \leq j+1 \\ 1 & \text{if } i = 1 \text{ and } j = 0 \\ 1-\alpha & \text{if } i = j = 0 \\ -g^{\alpha-1}_{n-i} & \text{if } j = n \text{ and } i \leq n \\ 0 & \text{otherwise .} \end{cases}$$

- $\beta^+ b_{i,j}$ is the rate of mass leaving from location x_i and arriving at x_j.
- The entries for column $j = 0$ prevent mass from leaving the left boundary $x = L$, while the entries for $j = n$ prevent mass from leaving the right boundary $x = R$.
- The iteration matrices for reflecting/absorbing and absorbing/reflecting BCs have all entries in the n-th column or zeroth column set to zero, respectively. For absorbing BCs, set columns $j = 0$ and $j = n$ to zero.

Consistency of BCs: Riemann-Liouville Flux

- We show the iteration matrix for Riemann-Liouville flux is consistent with reflecting BCs: $p\mathbb{D}_{L^+}^{\alpha-1}u(x,t) = q\mathbb{D}_{R^-}^{\alpha-1}u(x,t)$.
- The explicit update equation at $x = R$ ($j = n$) is

$$u(x_n, t_{k+1}) = u(x_n, t_k) - \frac{pC\Delta t}{h^\alpha}\sum_{i=0}^{n} g_{n-i}^{\alpha-1} u(x_i, t_k) + \frac{qC\Delta t}{h^\alpha}\left(u(x_{n-1}, t_k) + (1-\alpha)u(x_n, t_k)\right)$$

- This is equivalent to

$$h\frac{u(x_n, t_{k+1}) - u(x_n, t_k)}{\Delta t} = -\frac{pC}{h^{\alpha-1}}\sum_{i=0}^{n} g_{n-i}^{\alpha-1} u(x_i, t_k) + \frac{qC}{h^{\alpha-1}}\sum_{i=0}^{1} g_{1-i}^{\alpha-1}(x_{n+i-i}, t_k)$$

Consistency of BCs: Riemann-Liouville Flux

- As $h \to 0$,

$$\frac{1}{h^{\alpha-1}} \sum_{i=0}^{n} g_{n-i}^{\alpha-1} u(x_i, t_k) \to D_{L^+}^{\alpha-1} u(x, t_k) \text{ at } x = R$$

- The second term $h^{1-\alpha} \sum_{i=0}^{1} g_{1-i}^{\alpha-1} (x_{n+i-i}, t_k)$ is consistent with $D_{R^-}^{\alpha-1} u(x, t_k)$ at $x = R$ as $h \to 0$. See (Baeumer et al., 2018a) for details.
- Apply a similar argument at $x = L$, yielding

$$p\mathbb{D}_{L^+}^{\alpha-1} u(x, t) = q\mathbb{D}_{R^-}^{\alpha-1} u(x, t) \text{ for } x = L \text{ and } x = R$$

- Apply a similar argument to demonstrate consistency of boundary conditions for the Caputo flux.

Stability Analysis: Riemann-Liouville Flux

To prove stability, estimate the eigenvalues of the matrices A and M using the Gerschgorin circle theorem (Atkinson, 1989):

Lemma

The radii of the Gerschgorin circles of the matrix $B^+ = [b_{i,j}]$ are given by

$$r_i = \sum_{j=0, j\neq i}^{n} |b_{i,j}|$$

are given by

$$r_i = \begin{cases} \alpha - 1 & \text{if } i = 0 \\ \alpha & \text{if } 0 < i < n \\ 1 & \text{if } i = n, \end{cases}$$

while the radii of the Gerschgorin circles of the matrix $B^- = [b_{n-i,n-j}]$ are r_{n-j}.

Stability Analysis: Riemann-Liouville Flux

Theorem

The explicit Euler method (for Riemann-Liouville flux) subject to any combination of absorbing and reflecting BCs is stable if $\Delta t/h^{\alpha} \leq 1/(\alpha C)$ *over the region* $L \leq x \leq R$ *and* $0 \leq t \leq T$.

Proof.

For reflecting BCs, the radii of the Gerschgorin circles are

$$R_i = \begin{cases} \beta_+(\alpha - 1) + \beta_- & \text{if } i = 0 \\ \beta_+\alpha + \beta_-\alpha & \text{if } 0 < i < n \\ \beta_+ + \beta_-(\alpha - 1) & \text{if } i = n, \end{cases}$$

$$a_{i,i} = \begin{cases} 1 - \beta_+(\alpha - 1) - \beta_- & \text{if } i = 0 \\ 1 - (\beta_+ + \beta_-)\alpha & \text{if } 0 < i < n \\ 1 - \beta_+ - \beta_-(\alpha - 1) & \text{if } i = n. \end{cases}$$

□

Stability Analysis: Riemann-Liouville Flux

Proof.

Hence $a_{i,i} + R_i = 1$ for all i, while $a_{i,i} - R_{i,i} = 1 - 2R_i$. To ensure $|\lambda_i| \leq 1$ and stability, we require $1 - 2R_i \geq -1$, or $R_i \leq 1$. Since the largest R_i is $\alpha(\beta_+ + \beta_-)$, requiring

$$\alpha\left(\beta_+ + \beta_-\right) \leq 1.$$

The cases of absorbing/reflecting, reflecting/absorbing, and absorbing BCs are similar. □

Theorem

The implicit Euler method with Riemann-Liouville flux subject to any combination of absorbing and reflecting BCs for $1 < \alpha \leq 2$ is unconditionally stable for all Δt and any grid spacing h.

Plan

Kernel: One-Sided Diffusion Equation w/ RL Flux

- In the one-sided case ($p = 1$), the kernel $\ker\left(\mathbb{D}^{\alpha}_{-1^+}\right)$ of the Riemann-Liouville derivative on the interval $[-1, 1]$ is computed in (Baeumer et al., 2018a). Define $p^+_\alpha(x) = (1+x)^\alpha / \Gamma(1+\alpha)$.

$$u(x) = c_0 p^+_{\alpha-2}(x) + c_1 p^+_{\alpha-1}(x) \text{ where } c_0, c_1 \in \mathbb{R}$$

- To check, note that $\mathbb{D}^{\alpha}_{-1^+} u(x) = D^2_x I^{2-\alpha}_{-1^+} u(x)$. Since $I^{\beta}_{-1^+} p^+_\alpha(x) = p^+_{\alpha+\beta}(x)$,

$$I^{2-\alpha}_{-1^+} u(x) = c_0 + c_1 x,$$

  which is the kernel of the second derivative D^2_x.
- The only steady state solution on $[-1, 1]$ with a total mass of one that satisfies reflecting BCs is $u_\infty(x) = 2^{1-\alpha}(\alpha - 1)(1+x)^{\alpha-2}$.
- The steady-state is singular at the left end-point $x = -1$ and regular at the right end-point $x = 1$.

Kernel: One-Sided Diffusion Equation w/ RL Caputo Flux

- The kernel $\ker\left(\mathbf{D}^{\alpha}_{-1^+}\right)$ of the Patie-Simon derivative on the interval $[-1,1]$ is computed in (Baeumer et al., 2018a):

$$u(x) = c_0 p^+_{\alpha-1}(x) + c_1 \text{ where } c_0, c_1 \in \mathbb{R}$$

- To check, note that $u'(x) = c_0 p^+_{\alpha-2}(x)$ and $I^{2-\alpha}_{-1^+} p^+_{\alpha-2}(x)$ is a constant.
- The only steady state solution on $[-1,1]$ with a total mass of one that satisfies reflecting BCs is $u_\infty(x) = 1/2$.
- This solution is the same as the steady-state solution for the classical $(\alpha = 2)$ diffusion equation.

Two-sided Jacobi Polyfractonomials

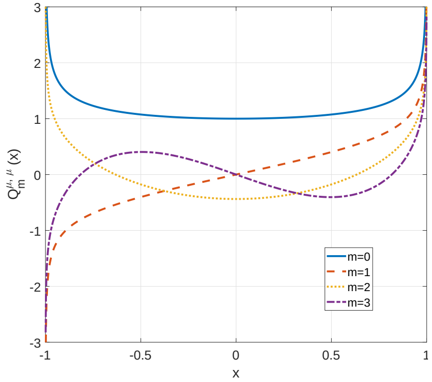


Figure: Two-sided Jacobi polyfractonomials ($m = 0, 1, 2$ and 3) with $\mu = \nu = -.25$.

Definition

The two-sided Jacobi polyfractonomials used by (Mao and Karniadakis, 2018) $Q_m^{\mu,\nu}(x)$ are defined by

$$Q_m^{\mu,\nu}(x) = (1-x)^{\mu}(1+x)^{\nu} P_m^{\mu,\nu}(x)$$

where $P_m^{\mu,\nu}(x)$ are Jacobi polynomials of order $m \geq 0$ and $\mu, \nu > -1$.

Fractional Integral of $Q_m^{\mu,\nu}(x)$

Lemma

Let $1 < \alpha < 2$, $p + q = 1$, *and let* $m \geq 0$ *be an integer. Using Theorem 6.4 in (Podlubny, 1999)*

$$pI_{-1^+}^{2-\alpha} Q_m^{\mu,\nu}(x) + qI_{1^-}^{2-\alpha} Q_m^{\mu,\nu}(x) = C_m P_m^{\nu,\mu}(x) \tag{9}$$

$$\mathcal{D}_{RL}^{\alpha} Q_m^{\mu,\nu}(x) = C_m \frac{\partial^2}{\partial x^2} P_m^{\nu,\mu}(x), \tag{10}$$

where

$$\mu + \nu = \alpha - 2$$

$$p - q = \cot\left(\pi\left(\frac{\alpha-1}{2} - \mu\right)\right)\tan\left(\frac{\alpha-1}{2}\pi\right)$$

$$C_m = \frac{\sin(\pi(\alpha-1)/2)\Gamma(m+\alpha-1)}{m!\sin(\pi(\alpha-1)/2 - \pi\mu)}.$$

Kernel: Two-Sided Riemann-Liouville Derivative

Theorem

The kernel of the two-sided Riemann-Liouville derivative on $[-1,1]$ *is given by*

$$\ker(\mathcal{D}_{RL}^{\alpha}) = c_0(1-x)^{\mu}(1+x)^{\nu} + c_1 x(1-x)^{\mu}(1+x)^{\nu}$$

where c_0 *and* c_1 *are arbitrary constants.*

Proof.

Let $m = 0$ or 1 in $\mathcal{D}_{RL}^{\alpha} Q_m^{\mu,\nu}(x) = C_m \frac{\partial^2}{\partial x^2} P_m^{\nu,\mu}(x)$. Then

$$\frac{\partial^2}{\partial x^2} P_m^{\nu,\mu}(x) = 0.$$

Since $P_m^{\nu,\mu}(x)$ is either a constant or a linear function, $\ker(\mathcal{D}_{RL}^{\alpha})$ follows. □

Two-Sided Fractional Diffusion: RL Steady-State

Theorem

The steady state solution with unit mass

$$u_\infty(x) = K(1-x)^\mu(1+x)^\nu$$

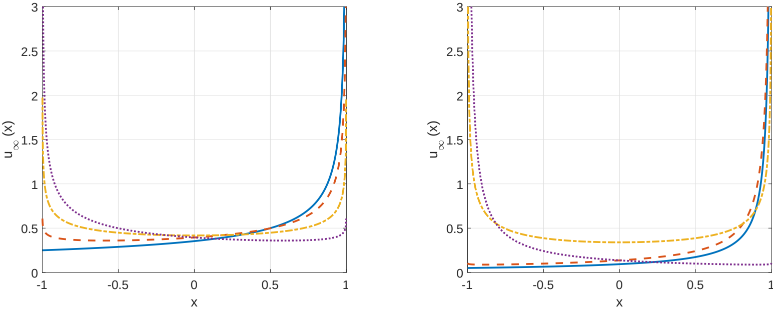
with normalization constant $1/K = B(\nu+1, \mu+1)2^{1+\mu+\nu}$ *satisfies* $\mathcal{D}^\alpha_{RL} u_\infty(x) = 0$ *subject to reflecting BCs*

$$p\mathbb{D}^{\alpha-1}_{-1^+} u(x,t) = q\mathbb{D}^{\alpha-1}_{1^-} u(x,t) \text{ for } x = L \text{ and } x = R \text{ for all } t \geq 0.$$

Proof.

Note that $u_\infty(x) = c_0 Q_0^{\mu,\nu}(x)$ satisfies the zero flux condition $F_{RL}(x,t) = -p\partial/\partial x I^{2-\alpha}_{-1^+} u_\infty(x) + q\partial/\partial x I^{2-\alpha}_{1^-} u_\infty(x) = 0$, while $c_1 Q_1^{\mu,\nu}(x)$ does not. □

Two-Sided Fractional Diffusion: RL Steady-State



(a) $\alpha = 1.5$ (b) $\alpha = 1.1$

Figure: Analytical steady state solution $u_\infty(x) = K(1-x)^\mu(1+x)^\nu$ evaluated using a) $\alpha = 1.5$ and and b) $\alpha = 1.1$ with $p = 0$ (solid), 0.25 (dashed), 0.5 (dash-dotted), and .75 (dotted).

Kernel of Two-Sided Patie-Simon Derivative

Theorem

The kernel of the two-sided Patie-Simon derivative $\mathcal{D}^{\alpha}_{PS}$ *on the interval* $[-1, 1]$ *is given by*

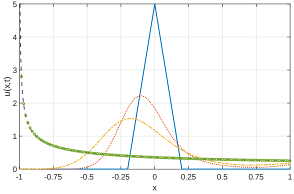
$$\ker(\mathcal{D}^{\alpha}_{PS}) = c_0 + c_1(1+x)^{1+\nu}{}_2F_1(-\mu, 1+\nu; 2+\nu; (1+x)/2). \quad (12)$$

where ${}_2F_1(a, b; c; w)$ *is the Gauss hypergeometric function. In particular, the steady state solution* $u_\infty(x)$ *subject to reflecting BCs with* $L = -1$ *and* $R = 1$ *with unit mass is* $u_\infty(x) = 1/2$.

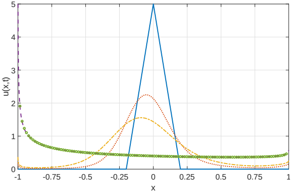
Remark

(Ervin et al., 2018) also computed the kernel of $\mathcal{D}^{\alpha}_{PS}$ *on* $[0, 1]$ *using a different method.*

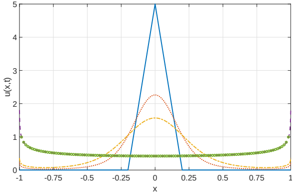
Numerical Experiments: Riemann-Liouville Flux



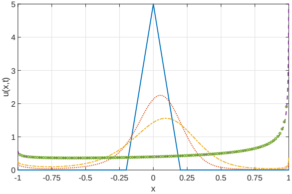
(a) p=1



(b) p=0.75



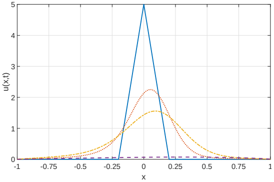
(c) p=0.5



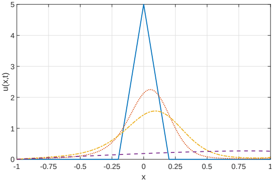
(d) p=0.25

Figure: Numerical solutions using $\alpha = 1.5$, $C = 1$, and reflecting BCs. $t = 0$ (solid), $t = 0.05$ (dotted), $t = 0.1$ (dash-dotted) and $t = 2$ (dashed), and the steady-state solution (circles).

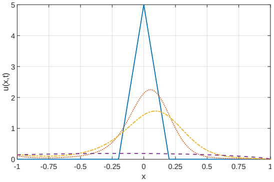
Numerical Experiments: Caputo Flux



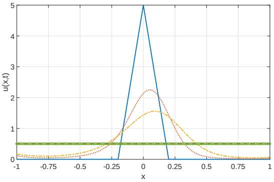
(a) absorbing



(b) absorbing-reflecting



(c) reflecting-absorbing



(d) reflecting

Figure: Numerical solutions using $\alpha = 1.5$, $C = 1$, and $p = 0.25$ using a) absorbing BCs, b) absorbing-reflecting BCs, c), reflecting-absorbing BCs, and d) reflecting BCs at $t = 0$ (solid), $t = 0.05$ (dotted), $t = 0.1$ (dash-dotted) and $t = 2$ (dashed).

Plan

Tempered Fractional Diffusion (w/ A. Lischke)

- The *normalized tempered fractional diffusion equation* is defined by

$$\frac{\partial}{\partial t} p_\lambda(x,t) = \mathbb{D}_+^{\alpha,\lambda} p_\lambda(x,t) - \lambda^\alpha p_\lambda(x,t) \tag{13}$$

  where $\lambda > 0$ is the tempering parameter and $1 < \alpha \leq 2$.

- The tempered Riemann-Liouville (TRL) derivative is defined by

$$\begin{aligned} \mathbb{D}_{L^+}^{\alpha,\lambda} f(x) &= e^{-\lambda x} \mathbb{D}_{L^+}^{\alpha} \left(e^{\lambda x} f(x) \right) \\ &= \frac{1}{\Gamma(2-\alpha)} \frac{d^2}{dx^2} \int_L^x e^{-\lambda(x-y)} (x-y)^{1-\alpha} f(y)\, dy, \end{aligned}$$

- Solutions on the real line are tempered α-stable densities $p_\lambda(x,t) = e^{\lambda x} p(x,t) e^{-t\lambda^\alpha}$ (Baeumer and Meerschaert, 2010).

Kernel of Tempered Fractional Diffusion Equation

- Determine all steady state-solutions $u_\infty(x)$ (e.g., kernel) of the one-sided tempered fractional diffusion equation on $[0,1]$:

$$\mathbb{D}_{0^+}^{\alpha,\lambda} u_\infty(x) - \lambda^\alpha u_\infty(x) = 0$$

- We utilize the *modified Mittag-Leffler functions* $E^*_{\alpha,\beta}(x)$ (Sankaranarayanan, 2014) and (Baeumer et al., 2018a):

$$E^*_{\alpha,\beta}(x) = x^\beta E_{\alpha,\beta+1}\left(x^\alpha\right) = \sum_{k=0}^{\infty} \frac{x^{k\alpha+\beta}}{\Gamma(\alpha k + \beta + 1)}$$

  where $E_{\alpha,\beta}(x)$ is the two-parameter Mittag-Leffler function (MLF).
- The modified Mittag-Leffler functions are eigenfunctions of the Riemann-Liouville derivative for $\beta = \alpha - 1$ and $\beta = \alpha - 2$

$$\mathbb{D}_{0^+}^{\alpha} E^*_{\alpha,\beta}(x) = E^*_{\alpha,\beta}(x)$$

Kernel of Tempered Fractional Diffusion Equation

Theorem

The tempered fractional diffusion equation has a kernel

$$u_\infty(x) = c_0 e^{-\lambda x} E^*_{\alpha,\alpha-1}(\lambda x) + c_1 e^{-\lambda x} E^*_{\alpha,\alpha-2}(\lambda x),$$

for $1 < \alpha < 2$ *where* c_0 *and* c_1 *are arbitrary real constants.*

Proof.

Choose $w(x)$ such that $u_\infty(x) = w(x)e^{-\lambda x}$. Then $\mathbb{D}^{\alpha,\lambda}_{0^+} u_\infty(x) - \lambda^\alpha u_\infty(x) = 0$ reduces to an *eigenvalue problem* on the interval $[0, 1]$

$$\mathbb{D}^{\alpha}_{0^+} w(x) = \lambda^\alpha w(x). \tag{14}$$

Use the scaling property of the fractional derivative $\mathbb{D}^{\alpha}_{0^+} f(\lambda x) = \lambda^\alpha \mathbb{D}^{\alpha}_{0^+} f(x)$, and both $w(x) = E^*_{\alpha,\alpha-1}(\lambda x)$ and $w(x) = E^*_{\alpha,\alpha-2}(\lambda x)$ satisfy the eigenvalue problem. □

Steady State Solution with Reflecting Boundary Conditions

Theorem

The steady-state solution with unit mass for all t is

$$u_\infty(x) = \frac{e^{-\lambda x}}{K}\left(E^*_{\alpha,\alpha-2}(\lambda x) - E^*_{\alpha,\alpha-1}(\lambda x)\right) \tag{15}$$

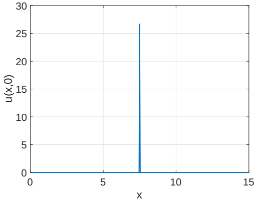
with normalization constant $K = e^{-\lambda}\lambda^{\alpha-2}E_{\alpha,\alpha}(\lambda^\alpha)$.

Proof.

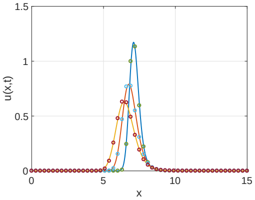
Let $u_0(x) = e^{-x}E^*_{\alpha,\alpha-1}(x)$ and $u_1(x) = e^{-x}E^*_{\alpha,\alpha-2}(x)$. By properties of MLFs, $u_1(x) > u_0(x)$ for all $x > 0$ and $u_0(x) \sim 1/\alpha$ and $u_1(x) \sim 1/\alpha$. Hence, the only choice c_0 and c_1 that ensures $u_\infty(x) = u_0(\lambda x) + u_1(\lambda x)$is non-negative for any λ is $c_1 = -c_0 = K > 0$. Then normalize via

$$K = \int_0^1 \left(u_1(x) - u_0(x)\right)\, dx$$

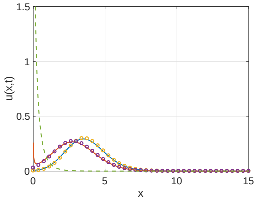
Numerical Solutions



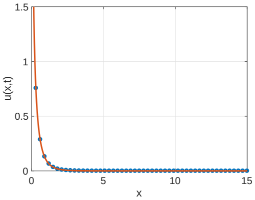
(a) $t = 0$



(b) $t = 0.2,\ 0.4,\ 0.6,\ 0.8$



(c) $t = 2.5$ and 3.0



(d) $t = 10$

Figure: Numerical solutions using $\alpha = 1.5$ and $\lambda = 1$. For b) short times, solutions are similar to $p_\lambda(x)$. For d) long times, numerical solution converges to $u_\infty(x)$.

Plan

Summary

- Reflecting (Neumann) boundary conditions for two versions of the two-sided, space-fractional diffusion equation that conserve mass were established.
- A conditionally stable explicit Euler scheme and an unconditionally stable implicit Euler scheme were proposed using the shifted Grünwald estimate from (Meerschaert and Tadjeran, 2004) and stability was demonstrated using the Gerschgorin circle theorem.
- Steady state solutions subject to reflecting BCs using Riemann-Liouville flux are singular at one or more of the end-points, while steady-state solutions subject to reflecting BCs using Caputo flux are constant functions.
- Steady-state solutions for (one-sided) tempered fractional diffusion were shown.

Open Problems

1. Explicitly compute the domains of the two-sided RL and PS fractional derivatives using the two-sided Jacobi polyfractonomials. Perhaps this can help establish well-posedness (in the strong sense) for two-sided fractional diffusion.
2. What is the correct flux/model/BC combination for a given application? Perhaps these 1D numerical models and steady-state solutions combined with **data** can help us pick out correct model for the application.
3. Applications to Hydrology and Fluid Mechanics: Adding an advection (drift) term and non-homogeneous BCs. Also need to formulate two-sided diffusion in 2D/3D with arbitrary boundaries.

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Caputo Fractional Diffusion is not a diffusion model!

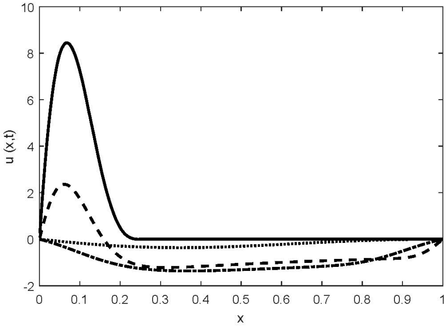


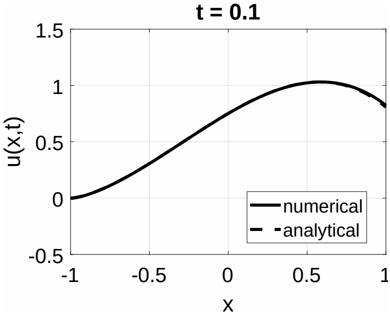
Figure: Numerical solution of the Caputo fractional diffusion equation with $\alpha = 1.5$.

Iteration Matrix: Caputo Flux

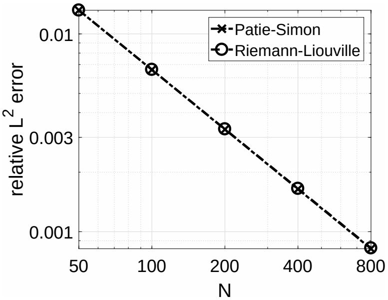
- Euler schemes associated with the Patie-Simon diffusion equation subject to reflecting BCs have an iteration matrix (Baeumer et al., 2018b)

$$b_{i,j} = \begin{cases} g^{\alpha}_{j-i+1} & \text{if } 0 < j < n \text{ and } i \leq j+1 \\ 1 & \text{if } i = 1 \text{ and } j = 0 \\ -1 & \text{if } i = j = 0 \\ -g^{\alpha-1}_{j} & \text{if } i = 0 \text{ and } 0 < j < n \\ -g^{\alpha-2}_{n-1} & \text{if } i = 0 \text{ and } j = n \\ -g^{\alpha-1}_{n-i} & \text{if } j = n \text{ and } 0 < i \leq n \\ 0 & \text{otherwise ,} \end{cases}$$

Numerical Experiment



(a) $n = 100$ grid points



(b) convergence study

Figure: Exact solution using the RL derivative ($n = 100$ grid points) and $\alpha = 1.5$ with $\beta = 2$. PS solution is very similar. b) relative L^2 error of the numerical solution.

$$u_0(x) = \frac{2^\beta}{1+\beta} p_\alpha^+(x) - \Gamma(1+\beta) p_{\alpha+\beta}^+(x). \tag{16}$$

$$s(x,t) = -e^{-t}\left(u_0(x) + \frac{2^\beta}{1+\beta} - \Gamma(\beta+1) p_\beta^+(x)\right), \tag{17}$$