Time Fractional Diffusion Equation

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Model problem:

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where $\Omega \subset \mathbb{R}^n$ is a smooth and bounded domain and $0 < \alpha \leq 1$.

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where $\Omega \subset \mathbb{R}^n$ is a smooth and bounded domain and $0 < \alpha \leq 1$.

$\rightarrow$ ${}_0^R\partial_t^\alpha$: Riemann-Liouville derivative

$\rightarrow$ ${}_0^C\partial_t^\alpha$: Caputo derivative

Riemann-Liouville Definition

- Left R.-L. fractional derivative of order $0 < \alpha \leq 1$ is defined as

$$
{}_0^R\partial_t^\alpha u(x,t) = \frac{1}{\Gamma(1-\alpha)} \frac{\partial}{\partial t} \int_0^t \frac{u(x,\tau)}{(t-\tau)^\alpha} \, d\tau,
$$

where $\Gamma(\cdot)$ denotes Gamma function

$$
\Gamma(x) = \int_0^\infty t^{x-1} e^{-t} \, dt
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$$ \Gamma(x) = \int_0^\infty t^{x-1} e^{-t} \, dt $$

- Right R.-L. fractional derivative of order $0 < \alpha \leq 1$ is defined as

$$ {}_t^R\partial_T^\alpha u(x,t) = -\frac{1}{\Gamma(1-\alpha)} \frac{\partial}{\partial t} \int_t^T \frac{u(x,\tau)}{(\tau-t)^\alpha} \, d\tau $$

Riemann-Liouville Definition

$\rightarrow$ Laplace transform of the R.-L. derivative ($n-1 \leq \alpha < n$)

$$\mathcal{L}\{{}_0^R D_t^\alpha f(t); s\} = s^\alpha \tilde{f}(s) - \sum_{k=0}^{n-1} s^k [{}_0^R D_t^{\alpha-k-1} f(t)]_{t=0},$$

Caputo Definition

- Left Caputo fractional derivative of order $0 < \alpha \leq 1$:

$$ {}_0^C\partial_t^\alpha u(x,t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial u(x,\tau)}{\partial \tau} \frac{1}{(t-\tau)^\alpha} \, d\tau $$

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$\rightarrow$ Laplace transform of the Caputo derivative ($n-1 < \alpha \leq n$)

$$ \mathcal{L}\{{}_0^C D_t^\alpha f(t); s\} = s^\alpha \tilde{f}(s) - \sum_{k=0}^{n-1} s^{\alpha-k-1} f^{(k)}(0), $$

Fractional Derivatives

Relationship between R.-L. and Caputio derivatives for $0 < \alpha \leq 1$:

$$
{}_{0}^{R}\partial_t^{\alpha} u(x,t) = \frac{u(x,0)}{\Gamma(1-\alpha)t^{\alpha}} + {}_{0}^{C}\partial_t^{\alpha} u(x,t)
$$

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- For homogeneous initial condition the R.-L. definition coincides with the Caputo definition
- R.-L. derivatives for definitions of new function classes
- Caputo derivatives for handling inhomogeneous initial conditions

Analytical Solution

1D time fractional diffusion equation for $0 < \alpha \leq 1$

$$
\begin{aligned}
{}_0^C\partial_t^\alpha u(x,t) - \partial_x^2 u(x,t) &= 0, \qquad x \in (0,1),\ t \geq 0 \\
u(0,t) = u(1,t) &= 0, \qquad t \geq 0 \\
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$\rightarrow$ separation of variables:

Analytical Solution

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\end{aligned}
$$

$\rightarrow$ separation of variables:

$$
u(x,t) = 2\sum_{k=1}^{\infty} E_{\alpha,1}(-(k\pi)^2 t^\alpha) sin(k\pi x) \int_0^1 u_0(\tau) sin(k\pi\tau)\, d\tau
$$

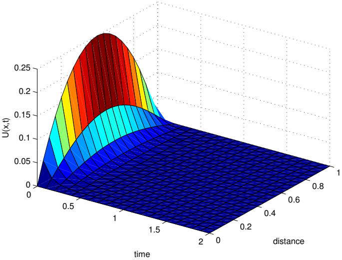
with Mittag-Leffler function

$$
E_{\mu,\nu}(z) := \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\mu k + \nu)}, \qquad z \in \mathbb{C}.
$$

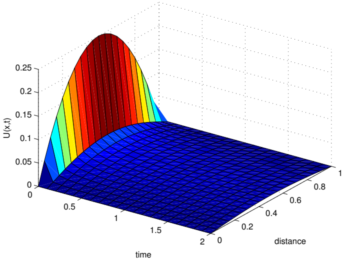
Example

$$u(x,t) = 2\sum_{k=1}^{\infty} E_{\alpha,1}(-(k\pi)^2 t^\alpha) sin(k\pi x) \int_0^1 u_0(\tau) sin(k\pi\tau)\, d\tau$$

$$u_0(x) = x(1-x), \qquad x \in (0,1)$$



solution for $\alpha = 1$



solution for $\alpha = \frac{1}{2}$

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Fractional Derivative Spaces [Ervin and Roop (2007)]

For $r, s > 0$ and $I = (0, T)$ we consider the anisotropic Sobolev spaces

$$H^{r,s}(\Omega \times I) = L^2(I; H^r(\Omega)) \cap H^s(I; L^2(\Omega))$$

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$$H^{r,s}(\Omega \times I) = L^2(I; H^r(\Omega)) \cap H^s(I; L^2(\Omega))$$

Define $H_l^s(I)$ as the closure of $C_0^\infty(I)$ with respect to the norm

$$\|v\|_{H_l^s(I)} := \left(\|v\|_{L^2(I)}^2 + |v|_{H_l^s(I)}^2\right)^{\frac{1}{2}}, \quad |v|_{H_l^s(I)} := \|{}_0^R D_t^s v\|_{L^2(I)}.$$

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$\rightarrow$ analogue we can define the spaces $H_r^s(I)$ and $H_c^s(I)$ with

$$|v|_{H_r^s(I)} := \|{}_t^R D_T^s v\|_{L^2(I)}$$

$$|v|_{H_c^s(I)} := |({}_0^R D_t^s v, {}_t^R D_T^s v)_{L^2(I)}|^{\frac{1}{2}}, \quad s \neq n - \frac{1}{2}$$

Properties

- For $s \neq n + \frac{1}{2}$ the spaces $H_c^s(I)$ and $H_0^s(I)$ are equal with seminorms and norms

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- For $0 < \alpha < 1$ and $w \in H^\alpha(I), v \in C_0^\infty(I)$:

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Properties

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- For $0 < \alpha < 1$ and $w \in H^1(I), w(0) = 0, v \in H^{\frac{\alpha}{2}}(I)$

$$\left({}_0^R D_t^\alpha w, v\right)_I = \left({}_0^R D_t^{\frac{\alpha}{2}} w, {}_t^R D_T^{\frac{\alpha}{2}} v\right)_I$$

Variational Formulation [Li and Xu (2010)]

Find $u \in H_0^{1,\frac{\alpha}{2}}(Q_T),\ u(x,0) = 0$:

$$\left({}_0^R\partial_t^{\frac{\alpha}{2}} u, {}_t^R\partial_T^{\frac{\alpha}{2}} v\right)_{Q_T} + (\partial_x u, \partial_x v)_{Q_T} = (f, v)_{Q_T}$$

for all $v \in H_0^{1,\frac{\alpha}{2}}(Q_T),\ v(x,0) = 0$ and $0 < \alpha < 1$.

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for all $v \in H_0^{1,\frac{\alpha}{2}}(Q_T),\ v(x,0) = 0$ and $0 < \alpha < 1$.

$\rightarrow$ Bilinearform is continuous and coercive

$\Rightarrow$ Existence and uniqueness of the solution by Lax-Milgram

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Model Problem

Time fractional diffusion equation with Caputo derivative

$$\begin{aligned} {}_0^C\partial_t^\alpha u - \Delta u &= 0, && \text{in } Q_T = \Omega \times (0, T), \\ u|_{\Sigma_T} &= g, && \text{on } \Sigma_T = \Gamma \times (0, T), \\ u(x, 0) &= 0, && \text{for } x \in \Omega, \end{aligned}$$

$0 < \alpha \leq 1$ and Ω open and bounded with smooth boundary.

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Consider the fractional diffusion equation

$$({}_0^C\partial_t^\alpha - \Delta) G(x,t) = \delta(x,t).$$

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$0 < \alpha \leq 1$ and Ω open and bounded with smooth boundary.

Consider the fractional diffusion equation

$$({}_0^C\partial_t^\alpha - \Delta)G(x, t) = \delta(x, t).$$

$\rightarrow$ Fourier-Laplace transform:

$$
\begin{aligned}
(|\xi|^2 + s^\alpha)\hat{\tilde{G}}(\xi, s) &= 1\\
\Leftrightarrow \qquad \hat{\tilde{G}}(\xi, s) &= \frac{1}{|\xi|^2 + s^\alpha}
\end{aligned}
$$

Fundamental Solution

Laplace transform of the Mittag-Leffler function:

$$\mathcal{L}\{t^{\nu-1}E_{\mu,\nu}(-\lambda t^{\mu}); s\} = \int_0^\infty e^{-st} t^{\nu-1} E_{\mu,\nu}(-\lambda t^{\mu})\, dt$$
$$= \frac{s^{\mu-\nu}}{s^{\mu}+\lambda}$$

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$\rightarrow$ Fourier transform of the fundamental solution:

$$\hat{\hat{G}}(\xi, s) = \frac{1}{|\xi|^2 + s^{\alpha}} \qquad \leftrightarrow \qquad \hat{G}(\xi, t) = t^{\alpha-1} E_{\alpha,\alpha}(-|\xi|^2 t^{\alpha})$$

Fundamental Solution

→ invert Fourier transform:

$$G(x,t) = (2\pi)^{-\frac{n}{2}} \int_{\mathbb{R}^n} t^{\alpha-1} E_{\alpha,\alpha}(-|\xi|^2 t^\alpha) e^{i\xi x}\, d\xi$$
$$= \pi^{-\frac{n}{2}} t^{\alpha-1} |x|^{-n} H_{(1)}\left(\frac{1}{4}|x|^2 t^{-\alpha}\right),$$

where

$$H_{(1)}(z) := H^{20}_{12}\left[z \,\middle|\, \begin{smallmatrix}(\alpha,\alpha)\\ (\frac{n}{2},1),(1,1)\end{smallmatrix}\right] = \frac{1}{2\pi i}\int_{\mathcal{C}} \frac{\Gamma(\frac{n}{2}+s)\Gamma(1+s)}{\Gamma(\alpha+\alpha s)} z^{-s}\, ds,$$

is the Mellin-Barnes integral definition of the Fox H-function

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Single Layer Potential

→ For a given boundary distribution $\sigma(x,t) \in C^\infty(\Sigma_T)$ we define the single layer potential

$$u(x,t) = S\sigma(x,t) = \int_0^t \int_\Gamma \sigma(y,\tau) G(x-y, t-\tau)\, ds_y\, d\tau,$$

for $x \in \Omega,\ t \in (0,T)$

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→ Boundary integral equation:

$$V\sigma(x,t) := \gamma(S\sigma)(x,t) = \gamma(u)(x,t) = g(x,t),$$

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→ For $0 < s < 1$ the operator

$$V : \tilde{H}^{-s,-\frac{\alpha}{2}s}(\Sigma_T) \to \tilde{H}^{1-s,\frac{\alpha}{2}(1-s)}(\Sigma_T)$$

is continuous

Jump Relations

Applying the time reversal operator $\kappa_T u(x,t) = u(x, T-t)$:

$$\int_0^T {}_0^C\partial_t^\alpha \varphi(t)\ (\kappa_T\psi)(t)\ dt = \int_0^T (\kappa_T\varphi)(t)\ {}_0^C\partial_t^\alpha \psi(t)\ dt$$

for $\varphi \in C^1([0,T])$ and $\psi \in C^1([0,T])$, $\psi(0) = 0$

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for $\varphi \in C^1([0,T])$ and $\psi \in C^1([0,T])$, $\psi(0) = 0$

$\rightarrow$ Green's formula for the fractional diffusion equation:

$$\int_{Q_T} \{({}_0^C\partial_t^\alpha - \Delta)u\ \kappa_T v - \kappa_T u\ ({}_0^C\partial_t^\alpha - \Delta)v\}\ dx\ dt$$
$$= \langle \gamma(u), \gamma_1(\kappa_T v)\rangle - \langle \gamma_1(u), \gamma(\kappa_T v)\rangle$$

for a smooth test function with $v(x,0) = 0$

Jump Relations [Kemppainen, Ruotsalainen (2010)]

$\Rightarrow$ For every $\psi \in H^{-\frac{1}{2},-\frac{\alpha}{4}}(\Sigma_T)$ there hold the jump relations

$$[\gamma(S\psi)] = 0,$$
$$[\gamma_1(S\psi)] = -\psi.$$

Coercivity

Theorem (Kemppainen, Routsalainen (2010))

The single layer operator $V : \tilde{H}^{-\frac{1}{2},-\frac{\alpha}{4}}(\Sigma_T) \to \tilde{H}^{\frac{1}{2},\frac{\alpha}{4}}(\Sigma_T)$ *is an isomorphism. Futhermore, it is coercive, i.e. there exists a positive constant c such that*

$$\langle V\sigma, \sigma \rangle \geq c \|\sigma\|^2_{H^{-\frac{1}{2},-\frac{\alpha}{4}}(\Sigma_T)}$$

for all $\sigma \in \tilde{H}^{-\frac{1}{2},-\frac{\alpha}{4}}(\Sigma_T)$*.*

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$$\langle V\sigma, \sigma \rangle \geq c \|\sigma\|^2_{H^{-\frac{1}{2},-\frac{\alpha}{4}}(\Sigma_T)}$$

for all $\sigma \in \tilde{H}^{-\frac{1}{2},-\frac{\alpha}{4}}(\Sigma_T)$.

$\to$ TFDE admits a unique solution $u(x,t) \in \tilde{H}^{1,\frac{\alpha}{2}}(Q_T)$

$$u(x,t) = S\sigma(x,t),$$

where $\sigma \in \tilde{H}^{-\frac{1}{2},-\frac{\alpha}{4}}(\Sigma_T)$ is the unique solution of

$$V\sigma = g, \qquad g \in \tilde{H}^{\frac{1}{2},\frac{\alpha}{4}}(\Sigma_T)$$

Outlook

- Investigation of the boundary integral operators

  $\rightarrow$ apply the theory of boundary integral equation to the fractional diffusion equation

- Behavior of the fundamental solution

- Space time discretizations for the time fractional diffusion equation

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Asymptotic Behavior [Kemppainen (2011)]

$$G(x,t) = \begin{cases} \pi^{-\frac{n}{2}} t^{\alpha-1} |x|^{-n} H_{(1)}\left(\frac{1}{4}|x|^2 t^{-\alpha}\right), & x \in \mathbb{R}^n, t > 0 \\ 0, & x \in \mathbb{R}^n, t > 0 \end{cases}$$

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(i) if $z := \frac{1}{4}|x|^2 t^{-\alpha} \geq 1$, then

$$|G(x,t)| \leq C t^{-\frac{\alpha n}{2} - 1 + \alpha} \exp(-\sigma t^{-\frac{\alpha}{2-\alpha}} |x|^{\frac{2}{2-\alpha}}),$$

where $\sigma = 4^{\frac{1}{\alpha-2}} \alpha^{\frac{\alpha}{2-\alpha}} (2-\alpha)$

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where $\sigma = 4^{\frac{1}{\alpha-2}} \alpha^{\frac{\alpha}{2-\alpha}} (2-\alpha)$

(ii) if $z \leq 1$, then

$$|G(x,t)| \leq C \begin{cases} t^{-1} & n = 2 \\ t^{-\frac{\alpha}{2}-1} & n = 3 \\ t^{-\alpha-1}(|\log(|x|^2 t^{-\alpha})| + 1) & n = 4 \\ t^{-\alpha-1}|x|^{-n+4} & n > 4 \end{cases}$$

Sarah-Lena Bonkhoff, Institut für Numerische Mathematik

Caputo Derivative

For $0 < \alpha < 1$ and $w \in H^1(I), v \in H^{\frac{\alpha}{2}}(I)$ we have

$$\left({}_0^C D_t^\alpha w, v\right)_I = \left({}_0^R D_t^{\frac{\alpha}{2}} w, {}_t^R D_T^{\frac{\alpha}{2}} v\right)_I - \left(\frac{w(0)t^{-\alpha}}{\Gamma(1-\alpha)}, v\right)_I .$$

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$\Rightarrow$ Variational Formulation: find $u \in H_0^{1,\frac{\alpha}{2}}(Q_T)$:

$$\left({}_0^R \partial_t^{\frac{\alpha}{2}} u, {}_t^R \partial_T^{\frac{\alpha}{2}} v\right)_{Q_T} + (\partial_x u, \partial_x v)_{Q_T} = (f, v)_{Q_T} + \left(\frac{u(x,0)t^{-\alpha}}{\Gamma(1-\alpha)}, v\right)_{Q_T}$$

for all $v \in H_0^{1,\frac{\alpha}{2}}(Q_T)$.

Continuity

Theorem (Kemppainen, Ruotsalainen (2010))

Let $0 < s < 1$. *The operator*

$$V : \tilde{H}^{-s,-\frac{\alpha}{2}s}(\Sigma_T) \to \tilde{H}^{1-s,\frac{\alpha}{2}(1-s)}(\Sigma_T)$$

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is continuous.

- $S\phi = G * \gamma'(\phi)$
- $\psi \mapsto G * \psi : \tilde{H}^{r,\frac{\alpha}{2}r}_{comp}(\mathbb{R}^n \times (0,T)) \to \tilde{H}^{r+2,\frac{\alpha}{2}(r+2)}_{loc}(\mathbb{R}^n \times (0,T))$ is continuous
- Trace $\gamma : H^{r,s}(Q_T) \to H^{\lambda,\mu}(\Sigma_T)$ is continuous and surjective for $\lambda = r - \frac{1}{2}, \mu = \frac{s}{r}\lambda$ and $r > \frac{1}{2}, s \geq 0$
- $\gamma' : H^{-\lambda,-\mu}(\Sigma_T) \to H^{-r,-s}_{comp}(\mathbb{R}^n \times (0,T))$