Finite Difference and Particle Methods for Fractional Diffusion Equations

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Journées Multiphasiques et Incertitudes, Nantes

Motivations

- Fractional diffusion phenomena in complex flows/media
  - droplets/bubbles in turbulent plumes
  - plumes in complex media (ocean, soil, . . .)
- Particle methods
  - ease of accounting for far field B.C.
  - low numerical diffusion
  - particularly suitable for advection-dominated transport
- Finite difference methods
  - non-constant diffusion coefficient (loss of coersivity in $H_0^{1-\beta/2} \times H_0^{1-\beta/2}$ of Galerkin approaches)
  - easier treatment of boundary conditions
  - extension to stochastic case
- UQ and Bayesian inference
  - uncertainty in fractional coefficient and diffusion coefficient
  - inference from data
  - design of experiments

Fractional diffusion

- general 1D diffusion equation :

$$\frac{\partial u(x,t)}{\partial t} = -\frac{\partial Q^\beta(x,t)}{\partial x}$$

- fractional diffusion flux $Q^\beta(x,t)$, **(Fickian for $\beta = 1$)**

$$Q^\beta(x,t) := -\frac{\mathcal{D}}{2\sin\beta\pi/2}\left[\frac{\partial^\beta u(x,t)}{\partial x^\beta} - \frac{\partial^\beta u(x,t)}{\partial(-x)^\beta}\right]$$

- Riemann-Liouville fractional derivative for $u(x,t)$ and $0 < \beta < 1$:

$$\frac{\partial^\beta}{\partial x^\beta} u(x,t) \equiv \frac{1}{\Gamma(1-\beta)} \frac{\partial}{\partial x} \int_{-\infty}^{x} \frac{u(\xi,t)}{(x-\xi)^\beta}\, d\xi$$

$$\frac{\partial^\beta}{\partial(-x)^\beta} u(x,t) \equiv \frac{-1}{\Gamma(1-\beta)} \frac{\partial}{\partial x} \int_{x}^{\infty} \frac{u(\xi,t)}{(\xi-x)^\beta}\, d\xi$$

- Fractional diffusion flux :

$$Q^\beta(x,t) = -\frac{\mathcal{D}}{2\sin(\beta\pi/2)\Gamma(1-\beta)} \frac{\partial}{\partial x} \int_{-\infty}^{\infty} \frac{u(\xi,t)}{|x-\xi|^\beta}\, d\xi$$

Riesz fractional derivative, fundamental solution and particle approximation

- For $\mathcal{D} = 1$ and $1 < \alpha = \beta + 1 < 2$, Riesz fractional derivative

$$\frac{\partial u(x,t)}{\partial t} \;:=\; {}_xD_0^{\alpha} u \;=\; \frac{\Gamma(\alpha)}{\pi(\alpha-1)} \sin\left(\frac{\alpha\pi}{2}\right) \frac{\partial^2}{\partial x^2} \int_{-\infty}^{\infty} \frac{u(\xi,t)}{|x-\xi|^{\alpha-1}}\, d\xi$$

- Fundamental solution [1] for $1 < \alpha < 2$:

$$\mathcal{G}_{\alpha}^{0}(x,t) = t^{\frac{-1}{\alpha}} \mathcal{L}_{\alpha}^{0}(t^{\frac{-1}{\alpha}} x), \quad \mathcal{L}_{\alpha}^{0}(x) = \frac{1}{x\pi} \sum_{n=1}^{\infty} (-x)^n \frac{\Gamma(1+n/\alpha)}{n!} \sin\left[\frac{-n\pi}{2}\right],$$

- Particle representation of $u(x,t)$:

$$u(x) = \sum_{i \in \mathcal{I}} V_i u_i \eta_{\epsilon}(x - x_i)$$

- V_i, u_i and ϵ : particle *volume*,*strength* and kernel width
- *kernel* $\eta_{\epsilon}(x - x_i)$: **[second order]**

$$\eta_{\epsilon}(x - x_i) = \frac{1}{\sqrt{\pi}\epsilon} \exp\left[-\left(\frac{x - x_i}{\epsilon}\right)^2\right]$$

1. F. Mainardi, Y. Luchko, G. Pagnini, The fundamental solution of the space-time fractional diffusion equation, Fractional Calculus and Applied Analysis, **4**, 153-192, (2001).

Direct differentiation method

- Inserting particle representation in Riemann-Liouville expression of Q^β, for $\mathcal{D} = 1$, gives

$$Q^\beta(x) = -\frac{2^{\frac{\beta-3}{2}}}{\sqrt{\pi}\epsilon^\beta \sin\left(\frac{\beta\pi}{2}\right)} \sum_{i\in\mathcal{I}} V_i u_i \frac{\partial}{\partial x}\left[\exp\left(-\frac{X_i^2}{4}\right)[D_{\beta-1}(-X_i) + D_{\beta-1}(X_i)]\right]$$

where $X_i \equiv \sqrt{2}(x - x_i)/\epsilon$ and D_ν denotes the parabolic cylinder function

- using the identity

$$\frac{\partial}{\partial x}\left[\exp\left(-\frac{x^2}{4}\right) D_\nu(x)\right] = -\exp\left(-\frac{x^2}{4}\right) D_{\nu+1}(x)$$

one obtains

$$Q^\beta(x) = -\frac{2^{\frac{\beta-2}{2}}}{\sqrt{\pi}\epsilon^{\beta+1} \sin\left(\frac{\beta\pi}{2}\right)} \sum_{i\in\mathcal{I}} V_i u_i \exp\left(-\frac{X_i^2}{4}\right)[D_\beta(-X_i) - D_\beta(X_i)] .$$

Direct differentiation method

- Similarly, differentiating the flux it comes

$$\frac{\partial Q^{\beta}(x)}{\partial x} = -\frac{2^{\frac{\beta-1}{2}}}{\sqrt{\pi}\epsilon^{\beta+2}\sin\left(\frac{\beta\pi}{2}\right)} \sum_{i\in\mathcal{I}} V_i u_i \exp\left(-\frac{X_i^2}{4}\right)\left[D_{\beta+1}(-X_i) + D_{\beta+1}(X_i)\right].$$

- discrete particle approximation

$$\frac{\partial u_i}{\partial t} = \frac{1}{\epsilon^{\alpha}} \sum_{j\in\mathcal{I}} V_j u_j G_{\epsilon}^{d}(x_i - x_j),$$

- radial kernel $G_{\epsilon}^{d}(r) = \frac{1}{\epsilon} G_{\alpha}^{d}\left(\frac{r}{\epsilon}\right)$ with

$$G_{\alpha}^{d}(r) = -\frac{2^{\frac{\alpha-2}{2}}}{\sqrt{\pi}\cos\left(\frac{\pi\alpha}{2}\right)} S^{\alpha+1}(r), \quad S^{\nu}(z) \equiv e^{-z^2/2}(D_{\nu-1}(-\sqrt{2}z)+D_{\nu-1}(\sqrt{2}z))$$

- **Non conservative**

Riemann-Liouville treatment

1 Start from

$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}\tilde{u}(x,t), \quad \tilde{u}(x,t) \equiv c_\beta \int_{-\infty}^{+\infty} \frac{u(\xi,t)}{|x-\xi|^\beta} \mathrm{d}\xi.$$

2 Inserting the particle representation of u it comes

$$\tilde{u}(x,t) = \frac{1}{\epsilon^{\beta-1}} \sum_{i\in\mathcal{I}} V_i u_i \kappa_\epsilon^\beta (x - x_i)$$

where $\kappa_\epsilon^\beta(r) = \frac{1}{\epsilon}\kappa^\beta\left(\frac{r}{\epsilon}\right)$ with

$$\kappa^\beta(r) = \frac{2^{\frac{\beta-3}{2}}}{\sqrt{\pi}\sin\left(\frac{\beta\pi}{2}\right)} S^\beta(r)$$

3 Evaluate Laplacian of $\tilde{u}(x,t)$ by PSE method

$$\frac{\partial u_i}{\partial t} = \frac{2}{\epsilon^2}\sum_{j\in\mathcal{I}} V_j(\tilde{u}_j - \tilde{u}_i)\Phi_\epsilon(x_j - x_i), \quad \Phi(r) = \frac{2}{\sqrt{\pi}}\exp(-r^2)$$

- Conservative method, but low decay of the Kernel $\kappa_\epsilon^\beta \sim x^{-\beta}$ for $x \to \infty$

Flux PSE method (FPSE)

1. Start from approximating the flux Q^β at the particle centers

$$Q_i^\beta = -\frac{1}{\epsilon^\beta} \sum_{j \in \mathcal{I}} V_j u_j F_\epsilon(x_i - x_j),$$

where

$$F(r) = \frac{2^{\frac{\beta-2}{2}}}{\sqrt{\pi} \sin\left(\frac{\beta\pi}{2}\right)} T^\alpha(r), \quad T^\nu(z) \equiv e^{\frac{-z^2}{2}} \left(D_{\nu-1}(-\sqrt{2}z) - D_{\nu-1}(\sqrt{2}z)\right)$$

2. Estimate the divergence of Q^β by PSE [2] :

$$\frac{\partial Q^\beta}{\partial x}(x_i) = \frac{1}{\epsilon} \sum_{j \in \mathcal{I}} V_j (Q_j^\beta + Q_i^\beta) \eta_\epsilon^1 (x_i - x_j)$$

3. Resulting in the particle scheme :

$$\frac{\partial u_i}{\partial t} = -\frac{1}{\epsilon} \sum_{j \in \mathcal{I}} V_j (Q_j^\beta + Q_i^\beta) \eta_\epsilon^1 (x_i - x_j), \qquad \eta^1(r) = -\frac{2r}{\sqrt{\pi}} \exp(-r^2)$$

[case of the first-derivative, full-space, second-order kernel]

2. J. D. Eldredge, A. Leonard, T. Colonius, A general deterministic treatment of derivatives in particle methods, *JCP*, **180** :2, 686-709, (2002)

Riesz treatment

- For $1 < \alpha < 2$ and $u \in C^2(\mathbb{R})$

$$ {}_xD_0^\alpha u(x) = \frac{\Gamma(1+\alpha)}{\pi} \sin\left(\frac{\alpha\pi}{2}\right) \int_0^\infty \frac{u(x+\xi) - 2u(x) + u(x-\xi)}{\xi^{1+\alpha}} \mathrm{d}\xi $$

- By change of variable

$$ {}_xD_0^\alpha u(x) = \frac{\Gamma(1+\alpha)}{\pi} \sin\left(\frac{\alpha\pi}{2}\right) \int_{-\infty}^\infty \frac{u(y) - u(x)}{|y-x|^{1+\alpha}} \mathrm{d}y. $$

- Considering

$$ u(x) \approx u_\epsilon(x) \equiv \int_{-\infty}^\infty u(z)\eta_\epsilon(x-z)dz, $$

- we got

$$ {}_xD_0^\alpha u(x) \approx {}_xD_0^\alpha u_\epsilon(x) = \frac{1}{\epsilon^\alpha} \int_{-\infty}^\infty u(z)G_\epsilon(x-z)dz, $$

with

$$ G_\epsilon(r) \equiv \frac{\Gamma(1+\alpha)}{\pi} \sin\left(\frac{\alpha\pi}{2}\right) \epsilon^\alpha \int_0^\infty \frac{\eta_\epsilon(r+\xi) - 2\eta_\epsilon(r) + \eta_\epsilon(r-\xi)}{\xi^{1+\alpha}} \mathrm{d}\xi $$

Same as the Direct Differentiation kernel.

Kernel PSE method (KPSE)

- For conservation we choose the template

$$\mathcal{I}(\epsilon, x) \equiv \frac{c}{\epsilon^\alpha} \int_{-\infty}^{\infty} (f(y) - f(x)) K_\epsilon(x-y)dy$$

with c a constant to be determine and K a smooth, radial kernel such that $\mathcal{I}(\epsilon, x) \to {}_xD_0^\alpha f$ as $\epsilon \to 0$

- a suitable choice is

$$K(r) = -\frac{1}{r}\frac{\partial \kappa^\beta}{\partial r}$$

- with corresponding KPSE scheme

$$\frac{\partial u_i}{\partial t} = \frac{\alpha}{\epsilon^\alpha} \sum_{j \in \mathcal{I}} V_j (u_j - u_i) K_\epsilon(x_j - x_i).$$

- Conservation is immediate.

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Green function treatment

- Recall the elementary solution

$$\mathcal{G}^0_\alpha(x,t) = \frac{1}{t^\gamma} L^0_\alpha\left(\frac{x}{t^\gamma}\right)$$

where $\gamma \equiv 1/\alpha$

- For $\Delta t > 0$ it comes

$$\begin{aligned} u(x,t+\Delta t) - u(x,t) &= \mathcal{G}^0_\alpha(x,\Delta t) * u(x,t) - u(x,t) \\ &= \int_{-\infty}^{\infty} \mathcal{G}^0_\alpha(x-y,\Delta t) u(y,t) \mathrm{d}y - u(x,t) \\ &= \int_{-\infty}^{\infty} \mathcal{G}^0_\alpha(x-y,\Delta t) \left[u(y,t) - u(x,t)\right] \mathrm{d}y. \end{aligned}$$

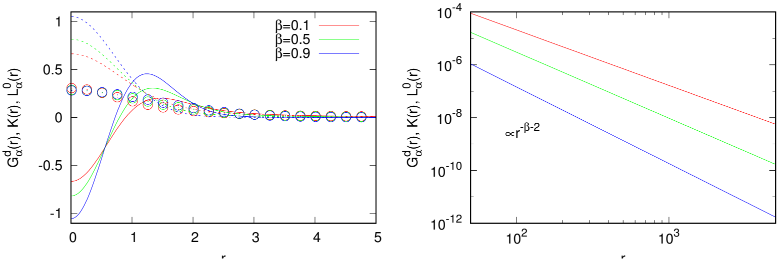
- or, setting $\Delta t = t^{n+1} - t^n$,

$$u_i^{n+1} - u_i^n = \sum_{j \in \mathcal{I}} V_j \left(u_j^n - u_i^n\right) E_\epsilon(x_j - x_i)$$

- with the GPSE radial kernel

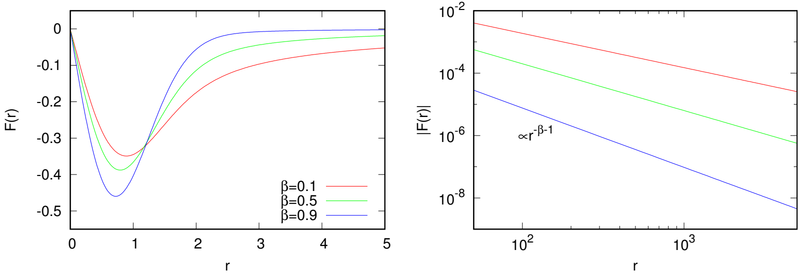
$$E(r) = L^0_\alpha(r), \quad \epsilon = (\Delta t)^\gamma$$

Kernels I



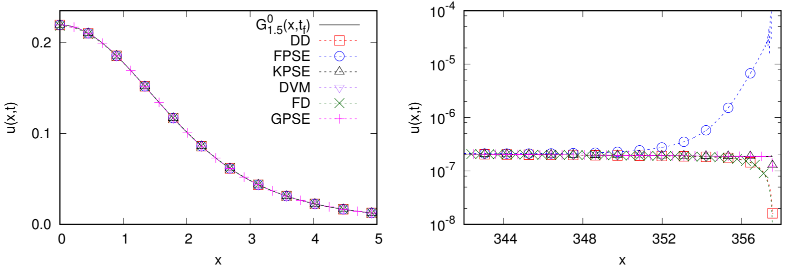
Kernels $G^d_\alpha(r)$ of direct differentiation (solid lines), $K(r)$ of KPSE method (dashed lines) and $L^0_\alpha(r)$ of GPSE (dotted lines)

Kernel II



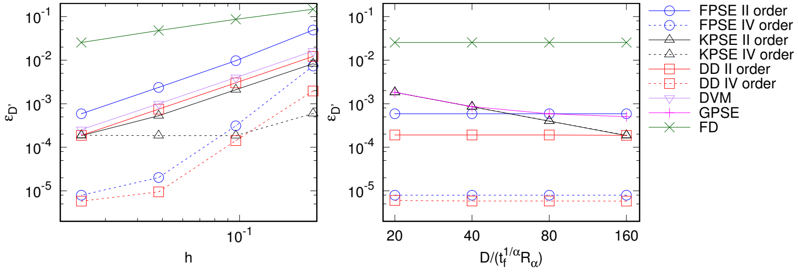
Kernel $F(r)$ of the flux reconstruction in FPSE.

Results I



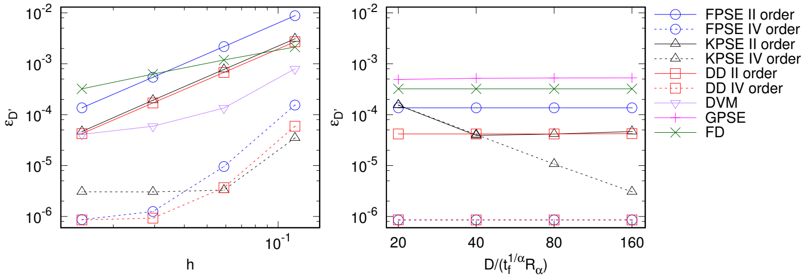
Fundamental solution at $t_f = 1.5$, for $\beta = 0.5$ and approximation by different methods.

Results II



Error at $t_f = 1.5$, for $\beta = 0.1$ as a function of particle volume h (left, with $D = 160 t_f^{1/\alpha} R_\alpha$) and domain truncation (right, with $h0.0121$).

Results III



Error at $t_f = 1.5$, for $\beta = 0.9$ as a function of particle volume h (left, with $D = 160 t_f^{1/\alpha} R_\alpha$) and domain truncation (right, with $h 0.0121$).

Results IV

β	$h \cdot 10^2$	DD		FPSE		KPSE		DVM
		II ord.	IV ord.	II ord.	IV ord.	II ord.	IV ord.	II ord.
0.1	4.83	2.01	3.88	2.04	3.97	1.98	3.79	2.00
0.5	4.46	2.00	3.97	2.01	3.86	2.00	4.06	2.00
0.9	5.89	2.00	4.00	2.01	3.96	2.00	3.99	2.42

Error at $t_f = 1.5$, reported convergence rate of the methods.

Fractional diffusion

- 1-d two-sided conservative fractional order differential equations with variable coefficient κ :

$$-\partial_x \left(\kappa(x)\partial_x^{\alpha,\theta} u(x)\right) = f(x), \quad \text{for } \; x \in \Omega := (a,b)$$

with $u(a) = u(b) = 0$.

- two-sided fractional order differential operator :

$$\partial_x^{\alpha,\theta}\phi := \theta \, {}_a\mathrm{D}_x^{\alpha}\phi + (1-\theta) \, {}_x\mathrm{D}_b^{\alpha}\phi$$

- left-sided (LS) and right-sided (RS) Riemann-Liouville fractional derivatives :

$${}_a\mathrm{D}_x^{\alpha} v(x) := \frac{\partial}{\partial x} \, {}_aI_x^{1-\alpha} v(x) = \frac{\partial}{\partial x}\int_a^x \omega_{1-\alpha}(x-z)v(z)\,dz$$

and

$${}_x\mathrm{D}_b^{\alpha} v(x) := \frac{\partial}{\partial x} \, {}_xI_b^{1-\alpha} = \frac{\partial}{\partial x}\int_x^b \omega_{1-\alpha}(z-x)v(z)dz$$

${}_aI_x^{1-\alpha}$ and ${}_xI_b^{1-\alpha}$ are the LS and RS Riemann-Liouville fractional integrals, with kernel $\omega_{1-\alpha}(x) := \frac{x^{-\alpha}}{\Gamma(1-\alpha)}$, where Γ is the gamma function.

Finite difference

- Partition of Ω in P subintervals $I_{1\leq n\leq P}$ using the sequence of $P+1$ points

$$a = x_0 < x_1 < x_2 < \cdots < x_P = b$$

- Uniform partition :

$$h = x_n - x_{n-1} = \frac{b-a}{P}$$

- $x_{n+1/2} := (x_n + x_{n+1})/2$ is the center of interval I_{n+1}
- Backward difference operator :

$$\delta v(x) = \delta v^n := v^n - v^{n-1}, \quad \forall x \in I_n$$

where $v^n := v(x_n)$

LS fractional derivative

For $\theta = 1$:

$$-\partial_x \left(\kappa(x) \, {}_a\mathrm{D}_x^\alpha u\right)(x) = f(x).$$

- forward type difference treatment of the operator ∂_x :

$$\partial_x \left(\kappa \, {}_a\mathrm{D}_x^\alpha u(x_n)\right) \approx h^{-1} \left[\kappa^{n+1/2} {}_a\mathrm{D}_x^\alpha u(x_{n+1}) - \kappa^{n-1/2} {}_a\mathrm{D}_x^\alpha u)(x_n)\right],$$

  where $\kappa^{n+1/2} := \kappa(x_{n+1/2})$

- Noting ${}_a\mathrm{D}_x^\alpha u = {}_aI_x^{1-\alpha} u'$, because $u(a) = 0$

$$\partial_x(\kappa \, {}_a\mathrm{D}_x^\alpha u)(x_n) \approx h^{-1}[\kappa^{n+1/2} {}_aI_x^{1-\alpha} u'(x_{n+1}) - \kappa^{n-1/2} {}_aI_x^{1-\alpha} u'(x_n)]$$

- backward difference approximation to the derivatives :

$$\partial_x(\kappa {}_a\mathrm{D}_x^\alpha u)(x_n) \approx h^{-2}[\kappa^{n+1/2}({}_aI_x^{1-\alpha}\delta u)(x_{n+1}) - \kappa^{n-1/2}({}_aI_x^{1-\alpha}\delta u)(x_n)]$$

Finite difference scheme for LS fractional derivative

$$
{}_aI_x^{1-\alpha}\delta u(x_n) = \sum_{j=1}^{n}\int_{I_j}\omega_{1-\alpha}(x_n - s)\delta u^j\, ds = \omega_{2-\alpha}(h)\sum_{j=1}^{n} w_{n,j}\delta u^j
$$

$$
= \omega_{2-\alpha}(h)\left(\sum_{j=1}^{n-1}[w_{n,j} - w_{n,j+1}]u^j + u^n\right),
$$

with the weights

$$
w_{n,j} := (n+1-j)^{1-\alpha} - (n-j)^{1-\alpha} \quad \text{for } n \geq j \geq 1.
$$

Denoting $U^n \approx u^n$ the finite difference solution, it comes

$$
\sum_{j=1}^{n}\left(a_{n,j} - a_{n+1,j}\right)U^j - \kappa^{n+1/2}U^{n+1} = \tilde{f}_h^n, \quad \text{for} \quad n = 1, \cdots, P-1
$$

where

$$
a_{n,j\leq n} = \begin{cases} \kappa^{n-1/2} & j = n, \\ \kappa^{n-1/2}[w_{n,j} - w_{n-1,j}] & j < n \end{cases}
$$

Finite difference scheme for LS fractional derivative

$$
\begin{aligned}
{}_aI_x^{1-\alpha}\delta u(x_n) &= \sum_{j=1}^{n}\int_{I_j}\omega_{1-\alpha}(x_n - s)\delta u^j\, ds = \omega_{2-\alpha}(h)\sum_{j=1}^{n} w_{n,j}\delta u^j \\
&= \omega_{2-\alpha}(h)\Big(\sum_{j=1}^{n-1}[w_{n,j} - w_{n,j+1}]u^j + u^n\Big),
\end{aligned}
$$

with the weights

$$
w_{n,j} := (n+1-j)^{1-\alpha} - (n-j)^{1-\alpha} \quad \text{for } n \geq j \geq 1.
$$

Denoting $U^n \approx u^n$ the finite difference solution, it solves $\mathbf{B}_L\mathbf{U} = \mathbf{F}$, where $\mathbf{U} = [U^1, U^2, \cdots, U^{P-1}]^T$, $\mathbf{F} = [\tilde{f}_h^1, \tilde{f}_h^2, \cdots, \tilde{f}_h^{P-1}]^T$, and the matrix $\mathbf{B}_L = [c_{n,j}]$ having **lower-triagonal entries**

$$
c_{n,j} = \begin{cases} \kappa^{n-1/2} - \kappa^{n+1/2}[2^{1-\alpha} - 2] & j = n, \\ a_{n,j} - a_{n+1,j} & j < n, \end{cases}
$$

while $c_{n,n+1} = -\kappa^{n+1/2}$

Finite difference scheme for LS fractional derivative

$\mathbf{B}_L\mathbf{U} = \mathbf{F}$, where $\mathbf{U} = [U^1, U^2, \cdots, U^{P-1}]^T$, $\mathbf{F} = [\tilde{f}_h^1, \tilde{f}_h^2, \cdots, \tilde{f}_h^{P-1}]^T$, and the matrix $\mathbf{B}_L = [c_{n,j}]$ having **lower-triagonal entries**

$$c_{n,j} = \begin{cases} \kappa^{n-1/2} - \kappa^{n+1/2}[2^{1-\alpha} - 2] & j = n, \\ a_{n,j} - a_{n+1,j} & j < n, \end{cases}$$

while $c_{n,n+1} = -\kappa^{n+1/2}$

- solution $\mathbf{U}$ exists and is unique
- truncature error

$$T_h^n = \partial_x(\kappa_a \mathrm{D}_x^\alpha u)(x_n) - \frac{1}{h^2}\left(\kappa^{n+1/2}({}_aI_x^{1-\alpha}\delta u)(x_{n+1}) - \kappa^{n-1/2}({}_aI_x^{1-\alpha}\delta u)(x_n)\right)$$

- we prove (for sufficient continuity of u)

$$T_h^n = O(h)(1 + (x_n - a)^{-\alpha}), \quad \text{for } 1 \le n \le P - 1.$$

- for $0 < \alpha < 1$, the truncation error T_h^n is of order h for x_n not too close to the left boundary $x = a$

Finite difference scheme for RS fractional derivative

Similarly, for $\theta = 0$, we obtain $\mathbf{B}_R\mathbf{U} = \mathbf{F}$, with the system matrix $\mathbf{B}_R = [d_{n,j}]$ **having upper-triagonal entries**

$$d_{n,j} = \begin{cases} -\kappa^{n-1/2} w_{j,n-1} + (\kappa^{n-1/2} + \kappa^{n+1/2}) w_{j,n} - \kappa^{n+1/2} w_{j,n+1}, & j > n, \\ \kappa^{n+1/2} - \kappa^{n-1/2}[2^{1-\alpha} - 2], & j = n, \end{cases}$$

while $d_{n+1,n} = -\kappa^{n+1/2}$

- solution $\mathbf{U}$ exists and is unique
- truncature error

$$T_h^n = \partial_x(\kappa\, {}_x\mathrm{D}_b^\alpha u)(x_n) - \frac{1}{h^2}\left(\kappa^{n+1/2}({}_xI_b^{1-\alpha}\delta u)(x_n) - \kappa^{n-1/2}({}_xI_b^{1-\alpha}\delta u)(x_{n-1})\right)$$

- we prove (for sufficient continuity of u)

$$T_h^n = O(h) + E^n, \quad \text{for } 1 \le n \le P-1.$$

  where

$$E^n = O(h)\omega_{1-\alpha}(\xi - x_{n-1}), \quad \text{for some } \xi \in I_P$$

- for $0 < \alpha < 1$, the truncation error T_h^n is of order h for x_n not too close to the right boundary $x = b$

Finite difference scheme for two sided fractional derivative

For $\theta \in [0, 1]$, $U^n \approx u^n$ solves

$$\kappa^{n-1/2}[\theta\, {}_aI_x^{1-\alpha}\partial U(x_n) + (1-\theta)\, {}_xI_b^{1-\alpha}\partial U(x_{n-1})] \\ - \kappa^{n+1/2}[\theta\, {}_aI_x^{1-\alpha}\partial U(x_{n+1}) + (1-\theta)\, {}_xI_b^{1-\alpha}\partial U(x_n)] = h^2 f^n,$$

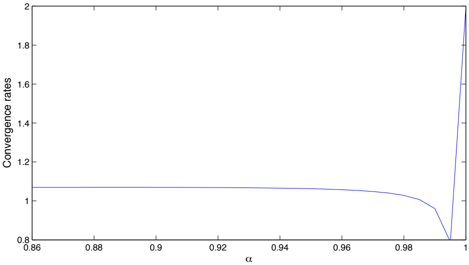
for $n = 1, \cdots, P-1$, and $U^0 = U^P = 0$.
The two sided fractional derivative system is

$$\mathbf{BU} = \mathbf{F}, \quad \mathbf{B} = \theta \mathbf{B}_L + (1-\theta)\mathbf{B}_R$$

Example I

Case of smooth solution in $\Omega = (0, 1)$ for $\kappa = 1 + \exp(x)$:

$$u_{\rm ex}(x) = x^{4-\theta(1-\alpha)}(1-x)^{4-(1-\theta)(1-\alpha)}$$



Convergence rate as a function of α for $\theta = 1/2$ and $P = 4192$

Example I

Case of smooth solution in $\Omega = (0,1)$ for $\kappa = 1 + \exp(x)$:

$$u_{\mathrm{ex}}(x) = x^{4-\theta(1-\alpha)}(1-x)^{4-(1-\theta)(1-\alpha)}$$

θ	$-\log_2 h$	$\alpha = 0.25$ E_h	$\alpha = 0.25$ σ_h	$\alpha = 0.50$ E_h	$\alpha = 0.50$ σ_h	$\alpha = 0.75$ E_h	$\alpha = 0.75$ σ_h
0.0	6	2.069e-04	0.9877	1.568e-04	0.9493	9.656e-05	0.8750
	7	1.040e-04	0.9929	8.028e-05	0.9659	5.164e-05	0.9030
	8	5.214e-05	0.9960	4.080e-05	0.9765	2.723e-05	0.9234
	9	2.611e-05	0.9976	2.064e-05	0.9834	1.421e-05	0.9382
	10	1.307e-05	0.9986	1.040e-05	0.9882	7.357e-06	0.9496
0.25	6	3.528e-04	0.9535	1.876e-04	0.9239	8.120e-05	0.8739
	7	1.784e-04	0.9838	9.622e-05	0.9636	4.275e-05	0.9255
	8	8.875e-05	1.0071	4.843e-05	0.9905	2.200e-05	0.9588
	9	4.325e-05	1.0369	2.393e-05	1.0173	1.108e-05	0.9887
	10	2.033e-05	1.0894	1.150e-05	1.0569	5.432e-06	1.0290
0.5	6	5.451e-04	0.8593	2.024e-04	0.8990	7.127e-05	8.7540
	7	2.865e-04	0.9280	1.045e-04	0.9530	3.705e-05	9.4381
	8	1.461e-04	0.9713	5.269e-05	0.9883	1.868e-05	9.8776
	9	7.289e-05	1.0036	2.599e-05	1.0198	9.157e-06	1.0287
	10	3.545e-05	1.0398	1.243e-05	1.0643	4.304e-06	1.0893
0.75	6	3.353e-04	0.9282	1.818e-04	0.9071	7.899e-05	0.8529
	7	1.714e-04	0.9672	9.392e-05	0.9527	4.190e-05	0.9147
	8	8.632e-05	0.9898	4.757e-05	0.9812	2.167e-05	0.9513
	9	4.289e-05	1.0092	2.370e-05	1.0054	1.097e-05	0.9820
	10	2.094e-05	1.0341	1.156e-05	1.0359	5.408e-06	1.0205
1.0	6	2.047e-04	0.9728	1.537e-04	0.9289	9.350e-05	0.8512
	7	1.034e-04	0.9855	7.929e-05	0.9546	5.048e-05	0.8893
	8	5.197e-05	0.9922	4.048e-05	0.9700	2.677e-05	0.9149
	9	2.607e-05	0.9956	2.053e-05	0.9794	1.403e-05	0.9326
	10	1.306e-05	0.9975	1.037e-05	0.9857	7.283e-06	0.9457

Example II

Case of non-smooth solutions in $\Omega = (0, 1)$ for $\kappa = 1 + \exp(x)$:

$$u_{\text{ex}}(x) = x^{1-\theta(1-\alpha)}(1-x)^{1-(1-\theta)(1-\alpha)}$$

		$\alpha = 0.25$		$\alpha = 0.50$		$\alpha = 0.75$	
θ	$-\log_2 h$	E_h	σ_h	E_h	σ_h	E_h	σ_h
0.0	7	5.057e-02	0.2752	1.916e-02	0.5123	4.624e-03	0.7626
	8	4.214e-02	0.2632	1.348e-02	0.5068	2.732e-03	0.7590
	9	3.527e-02	0.2567	9.510e-03	0.5037	1.618e-03	0.7556
	10	2.959e-02	0.2534	6.716e-03	0.5019	9.601e-04	0.7533
	11	2.485e-02	0.2517	4.745e-03	0.5010	5.702e-04	0.7518
	12	2.088e-02	0.2509	3.354e-03	0.5005	3.388e-04	0.7510
1.0	7	4.895e-02	0.2297	1.881e-02	0.4877	4.496e-03	0.7289
	8	4.145e-02	0.2399	1.336e-02	0.4940	2.692e-03	0.7402
	9	3.498e-02	0.2449	9.465e-03	0.4970	1.606e-03	0.7454
	10	2.946e-02	0.2475	6.700e-03	0.4985	9.562e-04	0.7478
	11	2.480e-02	0.2487	4.740e-03	0.4993	5.690e-04	0.7490
	12	2.086e-02	0.2494	3.352e-03	0.4996	3.384e-04	0.7495

Convergence in $O(h^{\alpha})$ (here $\theta = 1$).

Example II

Case of non-smooth solutions in $\Omega = (0, 1)$ for $\kappa = 1 + \exp(x)$:

$$u_{\text{ex}}(x) = x^{1-\theta(1-\alpha)}(1-x)^{1-(1-\theta)(1-\alpha)}$$

Adapted discretization with refinement parameter $\gamma \geq 1$: $x_i = (i/P)^\gamma$

	$\gamma = 2$		$\gamma = 3$		$\gamma = 4$	
$\log_2 P$	E_h	σ_h	E_h	σ_h	E_h	σ_h
6	2.300e-02		8.128e-03		2.871e-03	
7	1.628e-02	0.4988	4.838e-03	0.7484	1.438e-03	0.9976
8	1.151e-02	0.4996	2.878e-03	0.7495	7.194e-04	0.9992
9	8.140e-03	0.4998	1.711e-03	0.7498	3.597e-04	0.9997
10	5.756e-03	0.4999	1.018e-03	0.7499	1.800e-04	0.9999
11	4.070e-03	0.4999	6.051e-04	0.7499	8.994e-05	0.9999
12	2.878e-03	0.5002	3.600e-04	0.7500	4.497e-05	0.9998

Case of $\theta = 1$ and $\alpha = 0.25$.

Limsi

Uncertainty in fractional diffusion equation

1 Steady equation

$$-\partial_x \left(\kappa(x)\partial_x^{\alpha,\theta} u(x)\right) = f(x)$$

2 uncertainty in $\kappa(x)$

3 uncertainty in α, θ

4 probabilistic approach :

$$(\kappa(x,\omega), \alpha(\omega), \theta(\omega)) \in \mathcal{P}(W, \Sigma, \mu)$$

5 *a priori* analysis : **parameters considered independent**

- spectral expansion of $u(x, t, \kappa, \alpha, \theta)$: smoothness, existence of second moments,. . .
- balancing error.

Bayesian inference

1 A priori distribution of the parameter

$$\pi(\kappa, \alpha, \theta)$$

2 model predictions $\Phi : u \mapsto \mathbb{R}^m$ of the experimental observation y

3 likelihood of the experimental observation

$$\mathcal{L}(y|\kappa, \alpha, \theta)$$

4 Bayesian update

$$p(\kappa, \alpha, \theta|y) \propto \mathcal{L}(y|\kappa, \alpha, \theta)\pi(\kappa, \alpha, \theta)$$

- selection of the *a priori* distribution
- surrogate model to reduce computational cost
- selection of the observation Φ that best inform on the parameter
- model error

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