# Uncertainty quantification and Bayesian inference for fractional diffusion models

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# Fractional Diffusion Model

## Motivations

Many transport problems exhibits (at certain scales) non-normal diffusion, e.g. for complex phenomena such as

- dispersion in porous media
- dispersion in turbulent flows
- ...

## Fractional diffusion models

Needs for model to account for some non-normal effects in

- non-normal in space: **spatial-fractional diffusion**
- memory effects : **time-fractional diffusion**

## Objectives

- Propose uncertainty quantification methods for fractional diffusion
- Investigate resolution of inference problems (Bayesian)

## Table of content

## Space-fractional diffusion equation

(Stochastic) Space-Fractional Diffusion Equation

## Space-Fractional diffusion

- Deterministic general 1D diffusion equation in unbounded domain:

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

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

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

- 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:

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

## Riesz fractional derivative & fundamental solution

- For $\kappa = 1$ and $1 < \alpha = \beta + 1 < 2$, Riesz fractional derivative

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

- Fundamental solution*for $1 < \alpha < 2$ and $-\infty < x < +\infty$:

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

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).

- Infinite domains handled by particle methods: arbitrary order

S. Allouch, M. Lucchesi, OLM, K. Mustapha, and O.M. Knio. Particle Simulation of Fractional Diffusion Equations, Computational Particle Mechanics, 7, pp. 491-507, (2020).

## Steady Fractional diffusion

Consider the steady solution with fractional flux in a bounded domain.

- 1-d two-sided conservative fractional order differential equations with variable coefficient $\kappa$:

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

  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:

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

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

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

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## Solution method

Fractional operator discretization involves approximating integral (convolution):

- the convolution kernels have slow decay
- convergence of the discretization scheme is critical
- can be enhanced by using graded mesh (adapted at boundaries)
- yields **dense discrete operators**

Mustapha, Furati, Knio and OLM. A Finite Difference Method for Space-Fractional Differential Equations with Variable Diffusivity Coefficients, Communications on Applied Mathematics and Computation, 2, (2020).

Boukaram, Lucchesi, Turkiyyah, OLM, Knio and Keyes, Hierarchical Matrix Approximation for Space-Fractional Diffusion Equations, Computer Methods in Applied Mechanics and Engineering, 369, (2020).

S. Allouch, M. Lucchesi, OLM, K. Mustapha, and O.M. Knio. Particle Simulation of Fractional Diffusion Equations, Computational Particle Mechanics, 7, pp. 491-507, (2020).

Below, we focus on 1d (inverse) problems but for **uncertain $\alpha$ and $\kappa$**.

Hal-Zahrani, Lucchesi, Mustapha, OLM and Knio. Bayesian calibration of order and diffusivity parameters in a fractional diffusion equation, J. Physics Commu., 5:8, (2021).

## Experiment 1: uncertain $\alpha \sim U(0.1, 0.9)$

$$-\partial_x \kappa(x) \partial_x^{\alpha} u(x) = f(x), \quad a \leq x \leq b.$$

- fractional coefficient $\alpha \sim U(0.1, 0.9)$
- deterministic $\kappa(x)$ and forcings $f$ (distributed or localized)
- PC expansion in $\alpha$ of $u(x)$ (using Gauss quadrature)

$$u(x, \alpha) \approx \hat{u}(x, \alpha) := \sum_k u_k(x) \Psi_k(\alpha).$$

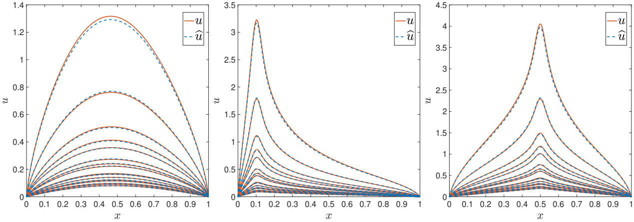


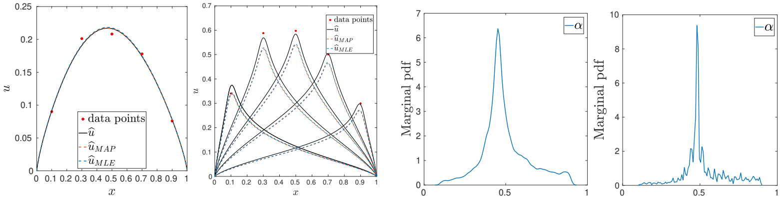

Figure 2: Case 1: solutions, $u$, and surrogates, $\widehat{u}$, for 16 randomly selected values of $\alpha$ corresponding to distributed forcing (left), localized forcing at $x_0 = 0.1$ (center) and at $x_0 = 0.5$ (right).

## Experiment 1: Bayesian Inference of $\alpha$

Learning $\alpha$ from observations (true value is 0.452)

- Use $n = 5$ noisy (Gaussian) observations $u(x_i)$
- Priors: $\boldsymbol{\alpha} \sim U(0.1, 0.9)$ and Jeffrey's for $\sigma_\epsilon$
- Bayesian posterior of $(\boldsymbol{\alpha}, \sigma_\epsilon)$

$$p(\alpha, \sigma_\epsilon | D) \propto \Pi_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma_\epsilon^2}} \exp\left(-\frac{(u_i - \hat{u}(x_i, \alpha))^2}{2\sigma_\epsilon^2}\right) \mathbb{I}_{[0.1,0.9]}(\alpha) \frac{1}{\sigma_\epsilon^2}$$



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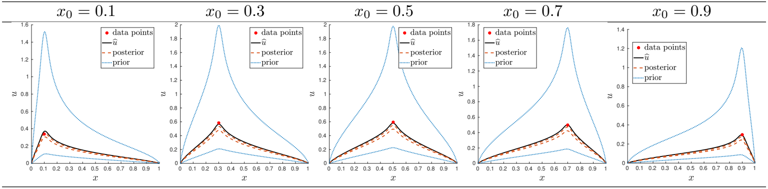



Figure 6: Case 1: profiles of the solution $\hat{u}$ for localized forcing setups, as indicated. Also plotted are curves showing the 95% bounds of the solution prior (blue dash) and the 50% bounds of the solution posterior (red dash). The noisy measurements used to perform the inference are also depicted. Note that a single inference step is performed using all five data points simultaneously.

# Experiment 2: log-normal $\kappa$

$$-\partial_x \boldsymbol{\kappa}(x)\partial_x^{\alpha} u(x) = f(x), \quad a \leq x \leq b.$$

- deterministic $\alpha = 0.5$ and forcings $f$ (distributed or localized)
- uncertain $\boldsymbol{\kappa}$ (with $\sigma_M = 0.5$ and $L_M = 0.75$)

$$\log \boldsymbol{\kappa}(x) \sim N(\mu, C(|x - x'|), \quad C(r) = \sigma_M^2 \exp(-(r/L_M)^2)$$

- truncated (5 modes) KL expansion: $\log \boldsymbol{\kappa}(x) \approx \mu + \sum_{l=1}^{5} \sqrt{\lambda_l}\Phi_l(x)\xi_l$
- PC expansion of $u(x, \boldsymbol{\xi})$ with LASSO from LHS with size 5,000 samples

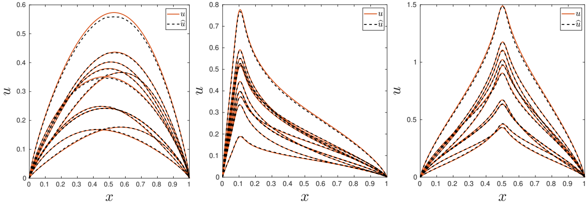


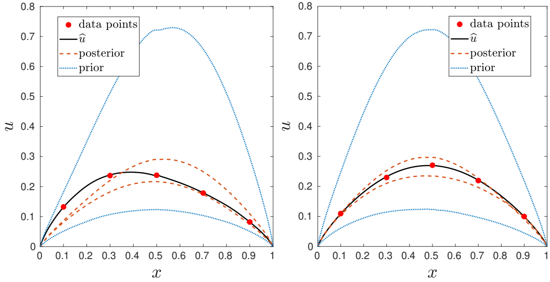

Figure 7: Case 2: solutions, $u$, and surrogates, $\widehat{u}$, considering distributed $f$ (left), and localized $f$ with $x_0 = 0.1$ (center) and $x_0 = 0.5$ (right). Simulations are performed using 10 randomly sampled values of $\boldsymbol{\xi}$. Surrogates are built using LASSO.

## Experiment 2: Inference of $\kappa$

Learn $\boldsymbol{\xi}$ in $\log \boldsymbol{\kappa}(x) \approx \mu + \sum_{l=1}^{5} \sqrt{\lambda_l}\Phi_l(x)\xi_l$

- Use $n = 5$ noisy (Gaussian) observations of $u(x)$ with Jeffrey's for $\sigma_\epsilon$
- Posterior of $(\boldsymbol{\xi}, \sigma_\epsilon)$ given by

$$p(\boldsymbol{\xi}, \sigma_\epsilon | D) \propto \Pi_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma_\epsilon^2}} \exp\left(-\frac{(u_i - \hat{u}(x_i, \boldsymbol{\xi}))^2}{2\sigma_\epsilon^2}\right) \mathbb{I}_{[0.1,0.9]}(\alpha) \frac{1}{\sigma_\epsilon^2}$$



## Experiment 2: Inference of $\kappa$

Learn $\xi$ in $\log \boldsymbol{\kappa}(x) \approx \mu + \sum_{l=1}^{5} \sqrt{\lambda_l}\Phi_l(x)\xi_l$

- Use $n = 5$ noisy (Gaussian) observations of $u(x)$ at 5 forcing points

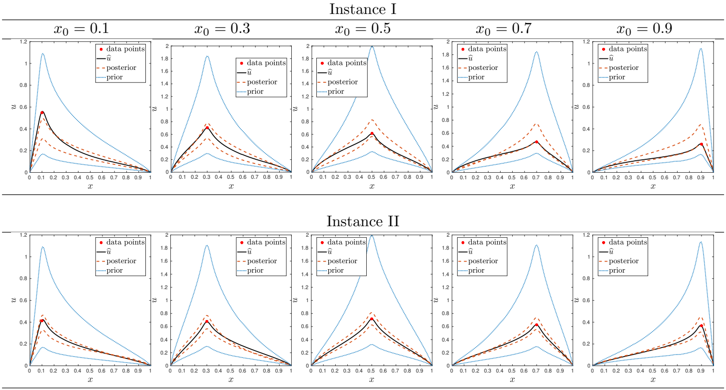



Figure 16: Case 2. Profiles of the solution, $u$, the 95% bounds of the pushed-forward prior (blue dash) and the 50% pushed-forward bounds of the posterior (red dash) of $\boldsymbol{\xi}$. The plots correspond to localized forcing experiments as indicated. Top row: Instance I; bottom row: Instance II. The noisy measurements used in the inference are also depicted.

# Experiment 3: Inference of $\kappa$ and $\alpha$

## Learn jointly $\boldsymbol{\alpha}$ and $\boldsymbol{\kappa}$

- PC model of $u(x, \alpha, \boldsymbol{\xi})$ constructed by PSP
- Use $n = 5$ noisy (Gaussian) observations of $u(x)$ at 5 points

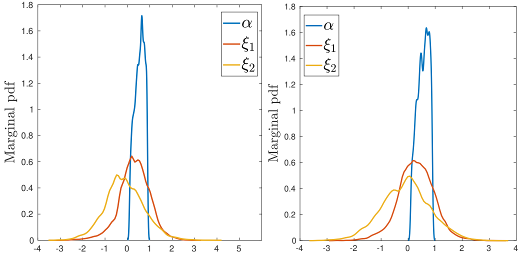



Figure 21: Case 3: marginal posterior of $\alpha$, $\xi_1$ and $\xi_2$ for distributed (left) and localized (right) forcing experiments.

# Experiment 3: Inference of $\kappa$ and $\alpha$

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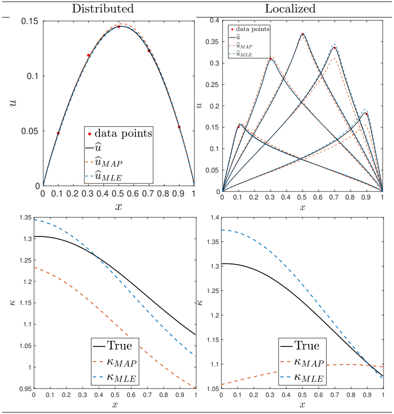

## Title-fractional diffusion equation

(Stochastic) Time-Fractional Diffusion Equation

## Title-fractional diffusion equation

We consider the time-fractional diffusion equation

$$\partial_t u(x,t) - \boldsymbol{\nabla} \cdot \left(\partial_t^{1-\alpha} \kappa \boldsymbol{\nabla} u\right)(x,t) = f(x,t), \quad \text{for } x \in \Omega \text{ and } 0 < t < T,$$

for $\Omega$ convex, polyhedral in $\mathbb{R}^d$ $(d \geq 1)$, completed with IC $u(x,0) = u_0(x)$ and homogeneous Dirichlet / Neumann BCs.

The fractional coefficient $\alpha \in (0,1]$ (case of $\alpha = 1$ correspond to normal diffusion).

We denote $\partial_t = \partial/\partial t$ the classical time partial derivative, and $\partial^{1-\alpha}/\partial t$ the time-fractional derivative (Riemann–Liouville sense):

$$\partial_t^{1-\alpha} v = \partial_t \mathcal{I}^\alpha v, \quad \mathcal{I}^\alpha v(t) = \int_0^t \omega_\alpha(t-s) v(s)\, ds \text{ with } \omega_\alpha(t) = \frac{t^{\alpha-1}}{\Gamma(\alpha)}, \quad \text{with } 0 < \alpha < 1.$$

The time-fractional derivative is a time-convolution (in the past).

## Time and space discretizations

L1 time-scheme: piecewise linear interpolation over a time mesh.

- Use a graded time-mesh with nodes $t_i$. Let $\gamma \geq 1$ and denote $N$ the number of time-intervals. We set

$$\tau = T^{1/\gamma}/N, \quad t_i = (i\,\tau)^\gamma, \quad \text{for } 0 \leq i \leq N.$$

  For $1 \leq n \leq N$, we denote $\tau_n = t_n - t_{n-1}$ the length of the $n$-th subinterval $I_n = (t_{n-1}, t_n)$.
- FE method for the spatial discretization: denote $V_h$ the FE space and $[\mathrm{D}_h]$ and $[\mathrm{M}_h]$ be the FE diffusion and mass matrices.
- The discretized problem writes

$$[\mathrm{M}_h](\mathrm{U}_h^n - \mathrm{U}_h^{n-1}) + \frac{\tau_n^\alpha}{\Gamma(\alpha+2)}[\mathrm{D}_h](\mathrm{U}_h^n + \alpha \mathrm{U}_h^{n-1}) = \mathrm{F}_h^n + \omega_{\alpha+1}(\tau_n)[\mathrm{D}_h]\mathrm{U}_h^{n-1}$$

$$-\left(\omega_{\alpha+1}(t_n) - \omega_{\alpha+1}(t_{n-1})\right)[\mathrm{D}_h]\mathrm{U}_h^0 - [\mathrm{D}_h]\sum_{j=1}^{n-1}\frac{\omega_{n,j}^\alpha}{\tau_j}(\mathrm{U}_h^j - \mathrm{U}_h^{j-1}), \quad \text{for } 1 \leq n \leq N,$$

  with
  $\omega_{n,j}^\alpha = \left(\omega_{\alpha+2}(t_n - t_{j-1}) - \omega_{\alpha+2}(t_{n-1} - t_{j-1})\right) - \left(\omega_{\alpha+2}(t_n - t_j) - \omega_{\alpha+2}(t_{n-1} - t_j)\right).$

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$$[\mathrm{S}_h^n]\mathrm{W}_h^n = \mathrm{F}_h^n - \left(\omega_{\alpha+1}(t_n) - \omega_{\alpha+1}(t_{n-1})\right)[\mathrm{D}_h]\mathrm{U}_h^0 - [\mathrm{D}_h]\sum_{j=1}^{n-1}\frac{\omega_{n,j}^\alpha}{\tau_j}\mathrm{W}_h^j, \quad \text{for } 1 \leq n \leq N,$$

where $[\mathrm{S}_h^n] = [\mathrm{M}_h] + \frac{\tau_n^\alpha}{\Gamma(\alpha+2)}[\mathrm{D}_h]$ and $\mathrm{W}_h^n = \mathrm{U}_h^n - \mathrm{U}_h^{n-1}$.

Mustapha, Knio and OLM, A second-order accurate numerical scheme for a time-fractional Fokker-Planck equation, IMA J. Numerical Analysis, (accepted).

# Case of stochastic $\alpha$

Let $\boldsymbol{\alpha}$ be random with density $p_{\boldsymbol{\alpha}}$ and satisfying $a < \boldsymbol{\alpha} < b$ a.s., for some $0 < a < b < 1$.
Let $\psi_{k=0,1,\dots}(\boldsymbol{\alpha})$, be mutually orthonormal random polynomials in $\boldsymbol{\alpha}$, where $\psi_k \in \pi_k$ (set of polynomials with degree $k$). The orthonormality conditions writes as

$$\mathbb{E}\left[\psi_k \psi_{k'}\right] = \int_a^b \psi_k(\alpha)\psi_{k'}(\alpha) p_{\boldsymbol{\alpha}}(\alpha) d\alpha = \delta_{kk'}.$$

Any function $\boldsymbol{h}(\boldsymbol{\alpha}) \in L_2(\Theta)$ has a Polynomial Chaos (PC) expansion,

$$\boldsymbol{h}(\boldsymbol{\alpha}) = \sum_{k \geq 0} h_k \psi_k(\boldsymbol{\alpha}),$$

where the $h_k$ are called the PC coefficients of $\boldsymbol{h}(\boldsymbol{\alpha})$.
In practice the PC expansion will be truncated to a finite order $\mathrm{No}$,

$$\boldsymbol{h}(\boldsymbol{\alpha}) \approx \widehat{\boldsymbol{h}}(\boldsymbol{\alpha}) = \sum_{k=0}^{\mathrm{No}} h_k \psi_k(\boldsymbol{\alpha}) = \boldsymbol{\psi}^{\mathrm{T}}(\boldsymbol{\alpha})\boldsymbol{h},$$

For instance, the **stochastic vector of increments** $\mathbf{W}_h^n(\boldsymbol{\alpha}) \in \mathbb{R}^{d_h} \times L_2(\theta)$ will be expanded in

$$\mathbf{W}_h^n(\boldsymbol{\alpha}) \approx \widehat{\mathbf{W}_h^n} = \sum_{k=0}^{\mathrm{No}} \left(\mathrm{W}_h^n\right)_k \psi(\boldsymbol{\alpha}), \quad \left(\mathrm{W}_h^n\right)_{k=0,\dots,\mathrm{No}} \in \mathbb{R}^{d_h}.$$

## Stochastic Galerkin problem

Inserting the PC expansion of $\mathbf{W}_h^n(\boldsymbol{\alpha})$ in the discrete system yields a stochastic residual vector $\mathbf{R}_h^n$:

$$[\mathbf{S}_h^n]\widehat{\mathbf{W}_h^n} - \mathrm{F}_h^n + \left(\boldsymbol{\omega}_{\boldsymbol{\alpha}+1}(t_n) - \boldsymbol{\omega}_{\boldsymbol{\alpha}+1}(t_{n-1})\right)[\mathrm{D}_h]\mathrm{U}_h^0 + [\mathrm{D}_h]\sum_{j=1}^{n-1}\frac{\boldsymbol{\omega}_{n,j}^{\boldsymbol{\alpha}}}{\tau_j}\widehat{\mathbf{W}_h^j} = \mathbf{R}_h^n.$$

We request the residual to be orthogonal to the stochastic space and obtain the system

$$\sum_{l=0}^{\mathrm{No}} \mathbb{E}\left[\psi_k[\mathbf{S}_h^n]\psi_l\right]\left(\mathrm{W}_h^n\right)_l = \delta_{k,0}\mathrm{F}_h^n - \mathbb{E}\left[\psi_k\left(\boldsymbol{\omega}_{\boldsymbol{\alpha}+1}(t_n) - \boldsymbol{\omega}_{\boldsymbol{\alpha}+1}(t_{n-1})\right)\right][\mathrm{D}_h]\mathrm{U}_h^0$$
$$- \sum_{j=1}^{n-1}\sum_{l=0}^{\mathrm{No}}\frac{1}{\tau_j}\mathbb{E}\left[\psi_k\boldsymbol{\omega}_{n,j}^{\boldsymbol{\alpha}}\psi_l\right][\mathrm{D}_h]\left(\mathrm{W}_h^j\right)_l, \qquad (1)$$

to be satisfied for $k = 0, \ldots, \mathrm{No}$ and $n = 1, \cdots, N$.

## Stochastic Galerkin system

For stochastic matrix $[\mathbf{S}_h^n]$ with deterministic $\kappa$, it comes

$$\mathbb{E}\left[\psi_k[\mathbf{S}_h^n]\psi_l\right] = [\mathrm{M}_h]\delta_{k,l} + [\mathrm{D}_h]c_{k,l}^n, \quad c_{k,l}^n \doteq \mathbb{E}\left[\frac{\tau_n^{\alpha}}{\Gamma(\alpha+2)}\psi_k\psi_l\right].$$

Let us define $[\mathrm{S}_h^n(k,l)] \doteq [\mathrm{M}_h]\delta_{k,l} + c_{k,l}^n[\mathrm{D}_h]$ and

$$w_k^{n,0} \doteq \mathbb{E}\left[\psi_k\left(\omega_{\alpha+1}(t_n) - \omega_{\alpha+1}(t_{n-1})\right)\right], \quad w_{k,l}^{n,j} \doteq \frac{1}{\tau_j}\mathbb{E}\left[\psi_k\omega_{n,j}^{\alpha}\psi_l\right].$$

The Stochastic Galerkin problem writes: for $k = 0, \ldots, \mathrm{No}$

$$\sum_{l=0}^{\mathrm{No}}[\mathrm{S}_h^n(k,l)]\left(\mathrm{W}_h^n\right)_l = \delta_{k,0}\mathrm{F}_h^n - \sum_{l=0}^{\mathrm{No}} w_k^{n,0}[\mathrm{D}_h]\mathrm{U}_h^0 - \sum_{j=1}^{n-1}\sum_{l=0}^{\mathrm{No}} w_{k,l}^{n,j}[\mathrm{D}_h]\left(\mathrm{W}_h^j\right)_l,$$

- Large linear system of coupling the PC coefficients of $\widehat{\mathrm{W}_h^n}$
- The Galerkin system is SPD wih size $(\mathrm{No}+1)d_h \times (\mathrm{No}+1)d_h$
- Iterative solvers (PCG): selection of preconditioners
- Evaluation of the coefficients $w_k^{n,0}$, $w_{k,l}^{n,j}$ and $c_{k,l}^n$

## Stochastic exponentiation

PC expansion of $\boldsymbol{h}(\alpha) = \tau^{\alpha}$ for $\tau > 0$. Since $\boldsymbol{h}(\alpha) = \exp(\alpha \log \tau)$ it is the solution $\boldsymbol{y}(t = 1)$ of the SODE

$$\frac{d\boldsymbol{y}}{dt} = \alpha \log \tau \, \boldsymbol{y}(t), \quad \boldsymbol{y}(t = 0) = 1.$$

For the PC expansion $\widehat{\boldsymbol{y}}(t) = \sum_{k=0}^{\mathrm{No}} y_k(t)\psi_k(\alpha)$ the Galerkin (weak) form of the SODE is

$$\frac{dy_k}{dt} = \log \tau \sum_{l=0}^{\mathrm{No}} \mathbb{E}\left[\psi_k \psi_l \alpha\right] y_l(t), \quad \text{for } k = 0, \ldots, \mathrm{No}.$$

Letting $\boldsymbol{y} = (y_0 \cdots y_{\mathrm{No}})^{\mathrm{T}}$ and $[\mathrm{A}_{\alpha}]_{k,l} = \mathbb{E}\left[\alpha \psi_k \psi_l\right]$, it comes

$$\frac{d\boldsymbol{y}}{dt} = (\log \tau)\,[\mathrm{A}_{\alpha}]\boldsymbol{y}, \quad \boldsymbol{y}(t = 0) = (1, 0, \cdots, 0)^{\mathrm{T}}$$

The matrix $[\mathrm{A}_{\alpha}]$ is SPD and can be decomposed in $[\mathrm{V}_{\alpha}][\Lambda][\mathrm{V}_{\alpha}]^{\mathrm{T}}$, with unitary $[\mathrm{V}_{\alpha}]$ and diagonal $[\Lambda]$. Denoting $\mathrm{l}$ the vector of eigenvalues ($\mathrm{l}_k = \lambda_k \geq 0$), we obtain

$$\tau^{\alpha} \approx \widehat{\tau^{\alpha}} = \psi(\alpha)^{\mathrm{T}}[\mathrm{V}_{\alpha}]\boldsymbol{v}(\tau), \quad \boldsymbol{v}_k(\tau) = \exp(\mathrm{l}_k \log \tau)[\mathrm{V}_{\alpha}]_{0,k} = \tau^{\mathrm{l}_k}[\mathrm{V}_{\alpha}]_{0,k}, \quad k = 0, \ldots, \mathrm{No}.$$

## Stochastic exponentiation (shifted case)

For latter use, consider a deterministic shift $s \in \mathbb{R}$. We have

$$[\mathrm{A}_{\alpha+s}] = [\mathrm{A}_{\alpha}] + s[\mathrm{I}] = [\mathrm{V}_{\alpha}]\left(\Lambda + s[\mathrm{I}]\right)[\mathrm{V}_{\alpha}]^{\mathrm{T}}.$$

Defining $\mathrm{l}(s)$ the vector of shifted eigenvalues, with $\mathrm{l}_k(s) = (\lambda_k + s)$, it comes

$$\tau^{\alpha+s} \approx \widehat{\tau^{\alpha+s}} = \psi(\alpha)^{\mathrm{T}}[\mathrm{V}_{\alpha}]\boldsymbol{v}(\tau, s), \quad \boldsymbol{v}_k(\tau, s) = \tau^{\mathrm{l}_k(s)}[\mathrm{V}_{\alpha}]_{0,k}, \quad k = 0, \dots, \mathrm{No}.$$

- Exponentiation requires the spectral decomposition of $[\mathrm{A}_{\alpha}]$
- $[\mathrm{A}_{\alpha}]$ depends only on $\alpha$ and the basis $(\mathrm{No})$
- cost of computing the PC expansion of $\tau^{\alpha+s}$ is $\mathrm{No}$ exponentials

## PC expansion of $\Gamma(\alpha)$

We now turn to the PC approximation of $\Gamma(\alpha)$. Recall

$$\Gamma(\alpha) = \int_0^{+\infty} \tau^{\alpha-1} e^{-\tau} d\tau.$$

Using the PC approximation of $\tau^{\alpha-1}$ (shift $s=-1$ above),

$$\tau^{\alpha-1} \approx \widehat{\tau^{\alpha-1}} = \psi(\alpha)^{T}[V_\alpha]\boldsymbol{v}(\tau,-1), \quad \boldsymbol{v}_k(\tau,-1) = \tau^{l_k(-1)}[V_\alpha]_{0,k}, \quad k=0,\dots,\mathrm{No},$$

and integrating we get the PC approximation of $\Gamma(\alpha)$:

$$\int_0^{+\infty} \psi(\alpha)^{T}[V_\alpha]\boldsymbol{v}(\tau,-1)e^{-\tau} d\tau = \psi(\alpha)^{T}[V_\alpha] \int_0^{+\infty} \boldsymbol{v}(\tau,-1)e^{-\tau} d\tau = \psi_k(\alpha)^{T}[V_\alpha]\boldsymbol{g}(-1),$$

where $\boldsymbol{g}(s)$ has for entries

$$\boldsymbol{g}_k(s) = [V_\alpha]_{0,k} \int_0^{+\infty} \tau^{l_k(s)} e^{-\tau} d\tau = [V_\alpha]_{0,k}\Gamma(l_k(s)+1), \quad k=0,\dots,\mathrm{No}.$$

We can generalize this approximation for some deterministic shift $s$:

$$\Gamma(\alpha+s) \approx \psi(\alpha)^{T}[V_\alpha]\boldsymbol{g}(s-1), \quad \boldsymbol{g}_k = [V_\alpha]_{0,k}\Gamma(l_k(s-1)+1).$$

## PC approximation of stochastic $\omega_{\alpha+s}(t)$

we consider the PC approximation of $\omega_{\alpha+s}$,

$$\omega_{\alpha+s}(t) = \frac{t^{\alpha+s-1}}{\Gamma(\alpha+s)} \approx \widehat{\omega_{\alpha+s}}(t) = \sum_{k=0}^{\mathrm{No}} h_k(t,s)\psi(\alpha).$$

Its PC coefficients $h_k$ are such that

$$\left(\psi(\alpha)^{\mathrm{T}}\boldsymbol{h}\right)\left(\psi(\alpha)^{\mathrm{T}}[\mathrm{V}_\alpha]\boldsymbol{g}\right) - \psi(\alpha)^{\mathrm{T}}[\mathrm{V}_\alpha]\boldsymbol{v} = \boldsymbol{r}(\alpha),$$

with $\mathbb{E}\left[\boldsymbol{r}\psi_k\right] = 0$ for $k = 0, 1, \dots, \mathrm{No}$. These conditions are equivalent to

$$[\mathrm{H}]\boldsymbol{h} = \boldsymbol{b}, \quad [\mathrm{H}]_{k,l} = \sum_{m=0}^{\mathrm{No}} C_{klm}\left(\sum_i [\mathrm{V}_\alpha]_{m,i}\boldsymbol{g}_i(s-1)\right), \quad \boldsymbol{b} = [\mathrm{V}_\alpha]\boldsymbol{v}(t,s),$$

The matrix $[\mathrm{H}]$ depends only on the shift $s$, when $\boldsymbol{b}$ is function of $s$ and $t$.
This enable the efficient PC approximation of the SFDE coefficients, for instance the rhs for $\omega^{\alpha}_{n,j}$ is

$$\boldsymbol{b}^{\alpha}_{n,j} = [\mathrm{V}_\alpha]\left(\boldsymbol{v}(t_n - t_{j-1}, 2) - \boldsymbol{v}(t_{n-1} - t_{j-1}, 2) - \boldsymbol{v}(t_n - t_j, 2) + \boldsymbol{v}(t_{n-1} - t_j, 2)\right).$$

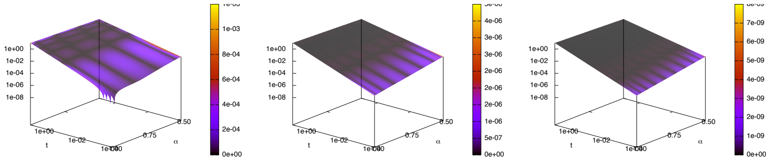
# Convergence of the PC approximations of the coefficients

Assume $\alpha$ has a uniform distribution $\mathcal{U}[a_{\min}, a_{\max}]$ and introduce $\xi \sim \mathcal{U}[0,1]$ to parametrize $\alpha(\theta)$ through

$$\alpha(\theta) = a_{\min} + (a_{\max} - a_{\min})\xi(\theta).$$

The random polynomials $\psi(\xi)$ are the normalized Legendre polynomials of the interval $[0,1]$.
Consider the PC approximation error

$$\epsilon_1 = \left| \widehat{\omega_{\alpha+1}(t)} - \omega_{\alpha+1}(t) \right|$$




(a) $n_o = 3$ (b) $n_o = 6$ (c) $n_o = 9$

Figure 1: Approximation $\widehat{\omega_{\alpha+1}(t)}$ for different PC order $n_o$. The color corresponds to the absolute error $|\widehat{\omega_{\alpha+1}(t)} - \omega_{\alpha+1}(t)|$. Case of $\alpha \sim \mathcal{U}[0.5, 1]$

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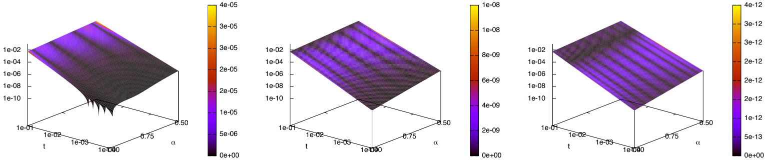


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Figure 2: Approximation $\widehat{\omega_{\alpha+2}(t)}$ for different PC order $n_o$. The color corresponds to the absolute error $|\widehat{\omega_{\alpha+2}(t)} - \omega_{\alpha+2}(t)|$. Case of $\alpha \sim \mathcal{U}[0.5, 1]$

## Convergence of the PC approximations of the coefficients

Assume $\boldsymbol{\alpha}$ has a uniform distribution $\mathcal{U}[a_{\min}, a_{\max}]$ and introduce $\boldsymbol{\xi} \sim \mathcal{U}[0,1]$ to parametrize $\boldsymbol{\alpha}(\theta)$ through

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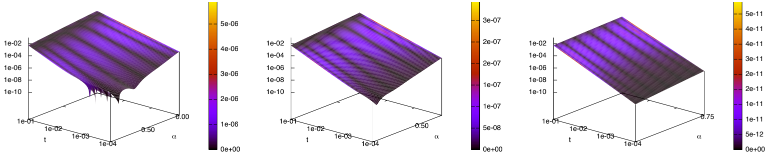
Consider the PC approximation error

$$\epsilon_1 = \left|\widehat{\boldsymbol{\omega}_{\boldsymbol{\alpha}+1}(t)} - \boldsymbol{\omega}_{\boldsymbol{\alpha}+1}(t)\right|$$




(a) $n_o = 6, \boldsymbol{\alpha} \sim \mathcal{U}[0,1]$ (b) $n_o = 6, \boldsymbol{\alpha} \sim \mathcal{U}[0.25,1]$ (c) $n_o = 6, \boldsymbol{\alpha} \sim \mathcal{U}[0.75,1]$

Figure 3: Approximation $\widehat{\boldsymbol{\omega}_{\boldsymbol{\alpha}+2}(t)}$ for PC order $n_o = 6$ and different uncertainty ranges. The color corresponds to the absolute error $|\widehat{\boldsymbol{\omega}_{\boldsymbol{\alpha}+2}(t)} - \boldsymbol{\omega}_{\boldsymbol{\alpha}+2}(t)|$.

# Convergence of the PC approximations of the coefficients

Assume $\alpha$ has a uniform distribution $\mathcal{U}[a_{\min}, a_{\max}]$ and introduce $\xi \sim \mathcal{U}[0,1]$ to parametrize $\alpha(\theta)$ through

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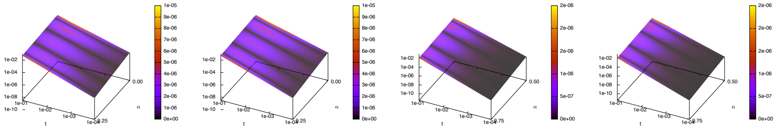
Consider the PC approximation error

$$\epsilon_1 = \left| \widehat{\omega_{\alpha+1}(t)} - \omega_{\alpha+1}(t) \right|$$

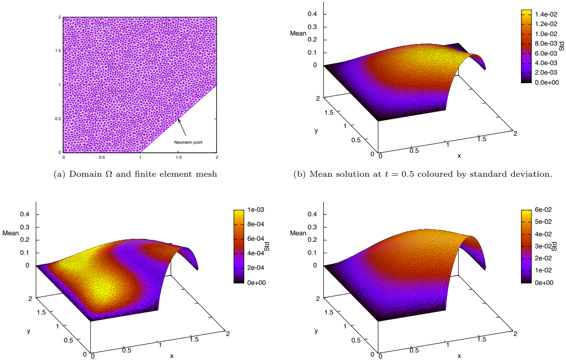


(a) $n_o = 3, \alpha \sim \mathcal{U}[0, 0.25]$ (b) $n_o = 3, \alpha \sim \mathcal{U}[0.25, 0.5]$ (c) $n_o = 3, \alpha \sim \mathcal{U}[0.5, 0.75]$ (d) $n_o = 3, \alpha \sim \mathcal{U}[0.75, 1]$

Figure 4: Approximation $\widehat{\omega_{\alpha+2}(t)}$ for PC order $n_o = 3$ and different uncertainty range having the same extend. The colo corresponds to the absolute error $|\widehat{\omega_{\alpha+2}(t)} - \omega_{\alpha+2}(t)|$.

CMAP

# Test Problem




(a) Domain Ω and finite element mesh

(b) Mean solution at $t = 0.5$ coloured by standard deviation.

(c) Mean solution at $t = 1.1$ coloured by standard deviation.

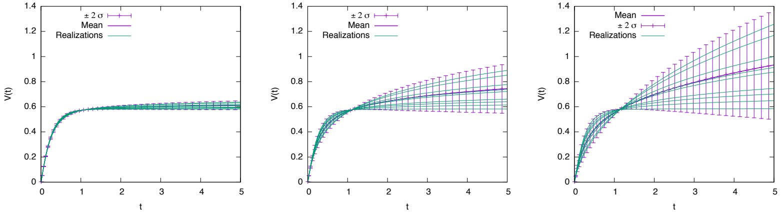
(d) Mean solution at $t = 5$ coloured by standard deviation.

Figure 5: Computational domain, finite element mesh and mean of the PC solution coloured by standard deviation value at different times as indicated. Case of $\boldsymbol{\alpha} \sim \mathcal{U}[0.75, 1]$, with PC expansions using $\mathrm{n_o} = 10$.

- Homogenous IC, uniform forcing: monotonic evolution to steady state
- Time mesh over $(0, 5]$ with 600 nodes and $\gamma = 1.2$
- FE mesh (P2) with 5,000 elements and 11,000 dof in space

# Test Problem

## Time evolutions at the center of the Neumann boundary



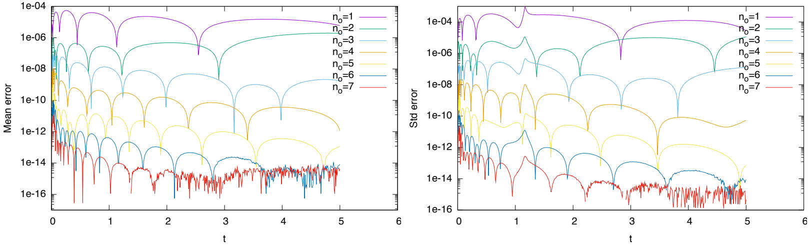

(a) $\boldsymbol{\alpha} \sim \mathcal{U}[0.95, 1]$ (b) $\boldsymbol{\alpha} \sim \mathcal{U}[0.75, 1]$ (c) $\boldsymbol{\alpha} \sim \mathcal{U}[0.5, 1]$

Figure 6: Solutions at the Neumann point (center of the Neumann boundary) for increasing range of $\boldsymbol{\alpha}$. The plots show the mean values of the PC approximation, with $\pm 2\sigma$ bounds, and a set of 10 random realizations of the PC expansion. Computation with $n_o = 10$. Other numerical parameters are provided in the text.

# Test Problem

Error on mean and Std at the center of the Neumann boundary:

$$\epsilon_{\text{mean}}(\text{No}) = |u_0 - \mathbb{E}[\boldsymbol{U}]|, \quad \epsilon_{\text{std}}(\text{No}) = \left| \left( \sum_{k=1}^{\text{No}} u_k^2 \right)^{1/2} - \mathbb{V}[\boldsymbol{U}]^{1/2} \right|,$$




(a) $\boldsymbol{\alpha} \sim \mathcal{U}[0.95, 1]$ (b) $\boldsymbol{\alpha} \sim \mathcal{U}[0.75, 1]$

Figure 7: Convergence with the PC order $n_o$ of the errors on the mean and standard deviation of $\widehat{\boldsymbol{U}_h}$ at the Neumann point. Case of $\boldsymbol{\alpha} \sim \mathcal{U}[0.5, 1]$

## Test Problem

### Integrated mean squared error:

$$\epsilon_{\mathrm{L2}}(t_n) = \mathbb{E}\left[\left(\mathbf{U}_h^n - \widehat{\mathbf{U}_h^n}\right)^{\mathrm{T}} [\mathrm{M}_h] \left(\mathbf{U}_h^n - \widehat{\mathbf{U}_h^n}\right)\right]^{1/2}.$$

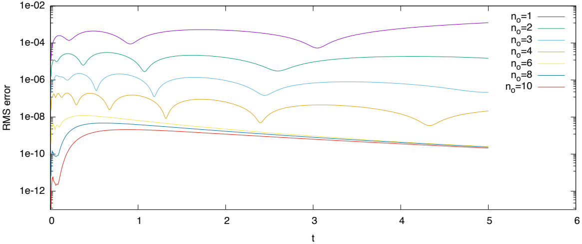



Figure 8: Convergence with the PC order $\mathrm{n_o}$ of the root mean squared error $\epsilon_{\mathrm{L2}}(t_n)$. Case of $\boldsymbol{\alpha} \sim \mathcal{U}[0.75, 1]$

# Conclusions and outlook

## Conclusions and Outlooks

### Summary

- Smooth dependences wrt to fractional and diffusion coefficients (space and time)
- Effective PC expansions with decent polynomial degree
- Design of experiments for fractional diffusion problems

### Outlooks

- Stochastic Galerkin methods for space-fractional equations
- Preconditioning of the Galerkin problems
- Hierarchical matrices for Galerkin problems
- Improved treatment of time-convolutions
- Spatially variable fractional coefficients

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