(2.) <u>Riemann-Liouville approach:</u>

Start with Cauchy n-fold integral formula

$$\frac{d^{-n}f(x)}{dx^{-n}} \equiv \int_a^x dx_{n-1} \int_a^{x_{n-1}} dx_{n-2} \cdots \int_a^{x_1} f(x_0)\,dx_0 = \frac{1}{(n-1)!}\int_a^x (x-x')^{n-1} f(x')\,dx'$$

Generalisation by introduction of the Γ function:
Riemann-Liouville fractional integral

$$ {}_a\mathcal{D}_{\cancel{x}}^{-\alpha} f(x) = \frac{1}{\Gamma(\alpha)} \int_a^x (x-x')^{\alpha-1} f(x')\,dx'$$

Fractional differentiation:

$$ {}_a\mathcal{D}_x^{\nu} f(x) = \left(\frac{d}{dx}\right)^n {}_a\mathcal{D}_x^{\nu-n} f(x) \quad :: \quad \nu>0, \quad n-1 \le \nu < n$$

<u>Examples:</u> (1.) Power-law function

$$ {}_0\mathcal{D}_x^{\alpha} x^p = \frac{d^n}{dx^n} {}_0\mathcal{D}_x^{-(n-\alpha)} x^p \overset{n-\alpha\equiv q}{=} \frac{d^n}{dx^n} \frac{1}{\Gamma(q)} \int_0^x (x-z)^{q-1} z^p\,dz$$

$$= \frac{d^n}{dx^n} \frac{1}{\Gamma(q)} \frac{\Gamma(q)\Gamma(p+1)}{\Gamma(q+p+1)} x^{q+p}$$

$$= \frac{\Gamma(p+1)}{\Gamma(p-\alpha+1)} x^{p-\alpha}$$ consistent with our heuristic generalisation

Here we used the Beta function integral

$$\int_0^x (x-x')^b x^d\,dt = \frac{\Gamma(b+1)\Gamma(d+1)}{\Gamma(d+b+2)} x^{b+d+1} = B(b+1,d+1)\,x^{b+d+1}$$

$$\forall \quad b>-1 \;\&\; d>-1.$$

(2.) Calculate ${}_0\mathcal{D}_x^{q} f(x) :: f(x) = x^{q-1} \sum_{j=0}^{\infty} \frac{x^{qj}}{\Gamma([1+j]q)} \quad :: 0<q\le 1$

$$ {}_0D_x^q f(x) = \cancel{\tfrac{d}{dx}} \sum_{j=0}^{\infty} \frac{1}{\Gamma([1+j]q)} \, {}_0D_x^q \, x^{q(1+j)-1} $$

$$ = \sum_{j=0}^{\infty} \frac{1}{\Gamma([1+j]q)} \frac{\Gamma(q[1+j])}{\Gamma(q[1+j]-q)} x^{qj-1} $$

$$ \Gamma(q[1+j]-q) \to \infty \ @ \ j=0 $$

$$ = \sum_{j=1}^{\infty} \frac{x^{qj-1}}{\Gamma(qj)} $$

$$ = \sum_{i=0}^{\infty} \frac{x^{q(i+1)-1}}{\Gamma(q[1+i])} = x^{q-1} \sum_{i=0}^{\infty} \frac{x^{qi}}{\Gamma([1+i]q)} \equiv f(x) $$

Thus $f(x)$ is a natural generalisation of the exponential function for fractional order differential equations.

$$ q=1: \quad f(x) = \sum_{i=0}^{\infty} \frac{x^i}{\Gamma(1+i)} = \sum_{i=0}^{\infty} \frac{x^i}{i!} = e^x. $$

Generalised Mittag-Leffler function:

$$ E_{\alpha,\beta}(z) = \sum_{j=0}^{\infty} \frac{z^j}{\Gamma(\alpha j+\beta)} $$

$$ \rightsquigarrow \quad f(x) = E_{q,q}(z^q). $$

<u>Fractional diffusion equation:</u>

We had previously in Laplace space for $\psi(t) \sim \tau^\alpha / t^{1+\alpha}$

$$ P(x,u) - \frac{\delta(x)}{u} = \frac{1}{u^\alpha} K_\alpha \frac{\partial^2}{\partial x^2} P(x,u) $$

The following theorem holds for fractional differentials:

$$\mathcal{L}\{ {}_0D_t^{-\alpha} f(t) \} = u^{-\alpha} f(u)$$

$$\Rightarrow \; P(x,t) - \delta(x) = {}_0D_t^{-\alpha} K_\alpha \frac{\partial^2}{\partial x^2} P(x,t)$$

equivalently:

$$\underline{\underline{\frac{\partial P(x,t)}{\partial t} = {}_0D_t^{1-\alpha} K_\alpha \frac{\partial^2}{\partial x^2} P(x,t)}} \quad \text{fractl. diffusion eq.}$$

Second moment:

$$\int x^2 \cdot dx \rightsquigarrow \frac{d}{dt}\langle x^2(t)\rangle = 2K_\alpha \, {}_0D_t^{1-\alpha} 1 = 2K_\alpha \frac{1}{\Gamma(\alpha)} t^{\alpha-1}$$

$$\rightsquigarrow \langle x^2(t)\rangle = \cancel{x_0^2} + 2K_\alpha t^\alpha \quad \checkmark$$

Can we relate the Brownian & the fractional propagators $P_1(x,t)$ & $P_\alpha(x,t)$?

We had the Fourier-Laplace form:

$$P_\alpha(k,u) = \frac{u^{\alpha-1}}{u^\alpha + K_\alpha k^2} \quad \text{for } \psi(t) \sim \tau^\alpha / t^{1+\alpha} \therefore \psi(u) \sim 1 - (u\tau)^\alpha$$

$$P_1(k,u) = \frac{1}{u + K_1 k^2}$$

$\Rightarrow$ we can relate the two PDFs by the rescaling relation

$$\underline{\underline{P_\alpha(k,u) = (u\tau)^{\alpha-1} P_1(k, u^\alpha \tau^{\alpha-1})}}.$$

This must also be valid for the inverse Fourier transform:

$$P_\alpha(x,u) = (u\tau)^{\alpha-1} P_1(x, u^\alpha \tau^{\alpha-1}).$$

We can write this relation as a generalised Laplace transform:

$$P_\alpha(x,t) = \int_0^\infty \mathcal{E}_\alpha(s,t)\, P_1(x,s)\, ds$$

$$\Big|\ \mathcal{L}\{P_\alpha(x,t);\ t\to u\}:\quad P_\alpha(x,u) = \int_0^\infty \mathcal{E}_\alpha(s,u)\, P_1(x,s)\, ds$$

$$\rightsquigarrow\ \mathcal{E}_\alpha(s,u) = u^{\alpha-1}\tau^{\alpha-1} e^{-su^\alpha\tau^{\alpha-1}} = -\frac{1}{\alpha s}\frac{d}{du} e^{-s\tau^{\alpha-1}u^\alpha}$$

$e^{-(u\tau)^\alpha}$ is the Laplace transform of the one-sided Lévy stable law

$$L_\alpha^+\left(\frac{t}{\tau}\right),\ \text{i.e.}\ \mathcal{L}\left\{L_\alpha^+\left(\frac{t}{\tau}\right)\right\} = e^{-(u\tau)^\alpha}.$$

$$\Rightarrow\ \mathcal{E}_\alpha(s,t) = \mathcal{L}^{-1}\left\{-\frac{1}{\alpha s}\frac{d}{du} e^{-s\tau^{\alpha-1}u^\alpha}\right\} = \frac{t}{\alpha s} L_\alpha^+\left(\frac{t}{(s\tau^{\alpha-1})^{1/\alpha}}\right)$$

using: $-\frac{d}{du} f(u) \xrightarrow{\mathcal{L}^{-1}} t f(t)$

for $\alpha = 1/2$ $\mathcal{E}_\alpha$ represents the Lévy-Smirnov law

$$\mathcal{E}_{1/2}(s,t) = \frac{1}{\sqrt{\pi t}}\, e^{-\frac{(s\tau^{-\frac{1}{2}})^2}{4t}} = \frac{1}{\sqrt{\pi t}}\, e^{-s^2/4\tau t}$$

The mapping from $P_1(x,t)$ to $P_\alpha(x,t)$ is called <u>subordination</u>, i.e., it corresponds to a transformation of the process time.

Representations using the subordination for certain values of α $(1/2, 1/3, \dots)$ are useful to plot the solution P_α based on the knowledge of P_1.

$\mathcal{E}_\alpha(s,t)$ is positive $\forall\ s,t>0 \Rightarrow$ The solution P_α is a proper PDF $\forall \alpha$.

Solution of the fractional diffusion equation:

There is no closed form solution involving simple functions. Here we consider the solution in terms of Fox H-functions (see, e.g., Metzler & Klafter, Phys Rep 339, 1 (20001).

Fourier invert $\mathcal{P}(k,u) = \dfrac{u^{\alpha-1}}{u^{\alpha}+K_\alpha k^2} \rightsquigarrow \mathcal{P}(x,u) = \dfrac{u^{\alpha/2-1}}{2K_\alpha^{1/2}} \exp\left(-\dfrac{|x|u^{\alpha/2}}{\sqrt{K_\alpha}}\right)$

The Fox function is defined through

$$H^{m,n}_{p,q}\left[z \left| \begin{matrix}(a_p, A_p)\\(b_q, B_q)\end{matrix}\right.\right] = H^{m,n}_{p,q}\left[z \left| \begin{matrix}(a_1,A_1),(a_2,A_2)\dots(a_p,A_p)\\(b_1,B_1)(b_2,B_2)\dots(b_q,B_q)\end{matrix}\right.\right] = \frac{1}{2\pi i}\int_L \chi(s)\, z^s\, ds :.$$

$$\chi(s) = \frac{\prod_1^m \Gamma(b_j - B_j s)\prod_1^n \Gamma(1-a_j+A_j s)}{\prod_{m+1}^q \Gamma(1-b_j+B_j s)\prod_{n+1}^p \Gamma(a_j - A_j s)}$$ with the properties

- $H^{m,n}_{p,q}\left[x \left| \begin{matrix}(a_p, A_p)\\(b_q, B_q)\end{matrix}\right.\right] = k\, H^{m,n}_{p,q}\left[x^k \left| \begin{matrix}(a_p, kA_p)\\(b_q, kB_q)\end{matrix}\right.\right]$

- $x^\sigma H^{m,n}_{p,q}\left[x \left| \begin{matrix}(a_p, A_p)\\(b_q, B_q)\end{matrix}\right.\right] = H^{m,n}_{p,q}\left[x \left| \begin{matrix}(a_p+\sigma A_p, A_p)\\(b_q+\sigma B_q, B_q)\end{matrix}\right.\right]$

- $z^b e^{-z} = H^{1,0}_{0,1}\left[z \left| \begin{matrix}\overline{}\\(b,1)\end{matrix}\right.\right]$

$$\Rightarrow \mathcal{P}(x,u) = \dots = \frac{|x|^{2/\alpha-1}}{2K_\alpha^{1/\alpha}} H^{1,0}_{0,1}\left[\frac{|x|u^{\alpha/2}}{\sqrt{K_\alpha}} \left| \begin{matrix}\overline{}\\(1-2/\alpha, 1)\end{matrix}\right.\right]$$

For $\mathcal{L}$: $$\mathcal{L}^{-1}\left\{H^{m,n}_{p,q}(u)\right\} = \frac{1}{t}\begin{cases} H^{n,m}_{q,p+1}\left[t \left| \begin{matrix}(1-b_q, B_q)\\(1-a_p, A_p),(1,1)\end{matrix}\right.\right], & 0 \le \mu \le 1 \\ H^{m,n}_{p+1,q}\left[\frac{1}{t} \left| \begin{matrix}(a_p, A_p),(0,1)\\(b_q, B_q)\end{matrix}\right.\right], & \mu \ge 1\end{cases}$$

$\mu = \sum B_q - \sum A_p$

The solution becomes:

$$P(x,t) = \frac{1}{\sqrt{4K_\alpha t^\alpha}} H^{1,0}_{1,1}\left[\frac{|x|}{\sqrt{K_\alpha t^\alpha}} \middle| \begin{matrix}(1-\alpha/2, \alpha/2)\\ (0,1)\end{matrix}\right]$$

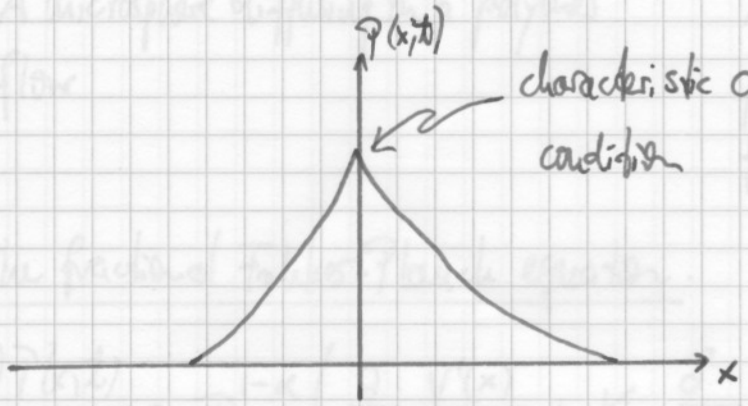
$$= \frac{1}{\sqrt{4K_\alpha t^\alpha}} \sum_{n=0}^{\infty} \frac{(-1)^n}{n!\,\Gamma(1-\alpha[n+1]/2)} \left(\frac{x^2}{K_\alpha t^\alpha}\right)^{n/2}$$

$$\sim \frac{1}{\sqrt{4\pi K_\alpha t^\alpha}} \sqrt{\frac{1}{2-\alpha}} \left(\frac{2}{\alpha}\right)^{(1-\alpha)/(2-\alpha)} \left(\frac{|x|}{\sqrt{K_\alpha t^\alpha}}\right)^{-(1-\alpha)/(2-\alpha)}$$

$$\times \exp\left(-\frac{2-\alpha}{2}\left(\frac{\alpha}{2}\right)^{\alpha/(2-\alpha)} \left[\frac{|x|}{\sqrt{K_\alpha t^\alpha}}\right]^{1/(1-\alpha/2)}\right)$$

$\frac{1}{1-\alpha/2} \in 1,2 \rightsquigarrow$ stretched Gaussian

$$\lim_{\alpha \to 1} P(x,t) = \frac{1}{\sqrt{4\pi K_1 t}} \exp\left(-\frac{x^2}{4K_1 t}\right) \checkmark$$



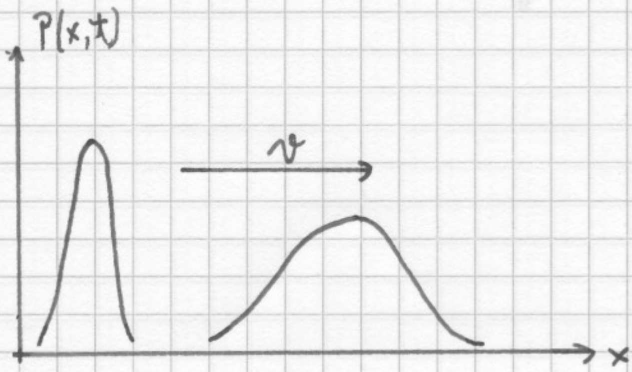
Fractional diffusion-advection equation:

Normal DAE: $$\frac{\partial P(x,t)}{\partial t} = -v\frac{\partial P}{\partial x} + K_1 \frac{\partial^2}{\partial x^2} P(x,t)$$

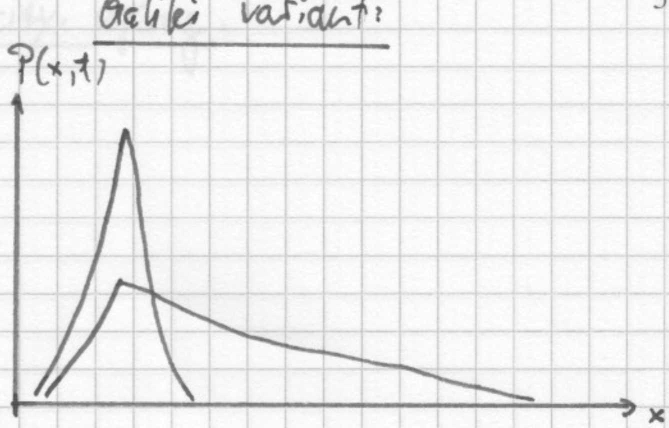
2 fractional variants: $$\frac{\partial P(x,t)}{\partial t} = -v\frac{\partial P}{\partial x} + {}_0D_t^{1-\alpha} K_\alpha \frac{\partial^2}{\partial x^2} P(x,t)$$ Galilei invariant

$$\frac{\partial P(x,t)}{\partial t} = {}_0D_t^{1-\alpha}\left(-v_\alpha\frac{\partial P}{\partial x} + K_\alpha \frac{\partial^2}{\partial x^2} P\right)$$ Galilei variant

Galilei invariant



Galilei variant:



$l \quad \langle x(t)\rangle = v t$

$\langle x^2(t)\rangle = \frac{2K_\alpha}{\Gamma(1+\alpha)} t^\alpha + v^2 t^2$

$\sigma^2 \quad \langle (\Delta x(t))^2\rangle = \frac{2K_\alpha}{\Gamma(1+\alpha)} t^\alpha$

$\frac{\sigma}{l} \sim \frac{t^{\alpha/2}}{t} \longrightarrow 0$

$\langle x(t)\rangle = \frac{v_\alpha t^\alpha}{\Gamma(1+\alpha)}$

$\langle x^2(t)\rangle = \frac{2v_\alpha^2 t^{2\alpha}}{\Gamma(1+2\alpha)} + \frac{2K_\alpha}{\Gamma(1+\alpha)} t^\alpha$

$$\langle (\Delta x(t))^2\rangle = \frac{2K_\alpha t^\alpha}{\Gamma(1+\alpha)} + \cancel{\frac{1}{\Gamma^2(1+\alpha)}} + \left(\frac{2}{\Gamma(1+2\alpha)} - \frac{1}{\Gamma^2(1+\alpha)}\right) v_\alpha^2 t^{2\alpha}$$

$\frac{\sigma}{l} \sim 1$

A microsphere diffusing in a polymer flow

A charged microsphere in a stationary polymer solution driven by an electrical field

The fractional Fokker-Planck equation.

$$\frac{\partial P(x,t)}{\partial t} = {}_0D_t^{1-\alpha}\left(\frac{\partial}{\partial x}\frac{V'(x)}{m\eta_\alpha} + K_\alpha \frac{\partial^2}{\partial x^2}\right) P(x,t)$$

$P_{st}(x) = N \exp\left(-\frac{V}{m\eta_\alpha K_\alpha}\right) \rightsquigarrow K_\alpha = \frac{k_B T}{m\eta_\alpha}$ generalised Einstein-Stokes

$\langle x(t)\rangle_{F_0} = \frac{F_0}{2k_B T}\langle x^2(t)\rangle_0$ generalised 2^{nd} Einstein relation

Both relations are experimentally verified.