

Fractional Partial Differential Equation: Introduction and Model

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- Diffusion describes the random movement of tracer particles from high concentration to low concentration.
- Two fundamental approaches were used to model diffusion.
- A deterministic/macroscopic description via a second-order diffusion PDE for the PDF of particle movements:
 - Fick set up the diffusion equation (1855) when studying how nutrients travel through membranes in living organisms, by mimicking the heat conduction equation of Fourier (1822).
 - Einstein derived the diffusion equation from first principles as part of his work on Brownian motion (1905).
- A stochastic/microscopic description via random walk of particles
 - Brown observed and investigated irregular movement of small pollen grain under a microscope (1827).
 - Pearson modeled a diffusion process in terms of random walk, when he studied on how mosquitoes spread malaria (1905).
 - Bachelier used a Brownian motion to model asset prices (1900).

- The common assumptions of Einstein and Pearson
 - the existence of a mean free path,
 - the existence of a mean waiting time to perform a jump.
- Under these approximations
 - Pearson's approach of random walk yields Brownian motion, which then leads to stochastic differential equation and is suited for a microscopic description of diffusive transport.
 - Einstein's derivation yields a Fickian diffusion equation, which can be viewed as a Fokker-Planck equation of Brownian motion.

- Let X be a random variable, $F(x) = \mathbb{P}[X \leq x]$ and $p(x) = F'(x)$ be its CDF and PDF, respectively, and $\mu_q = \mathbb{E}[X^q]$ be its q th moment.
- The common assumptions of Einstein and Pearson state the variance and mean waiting time of a randomly selected particle's motion are finite.
- If $\mu_1 = 0, \mu_2 = \sigma^2 < \infty$, the FT \hat{p} has the expansion

$$\begin{aligned}\hat{p}(k) &= \mathbb{E}[e^{-ikX}] = \int_{\mathbb{R}} e^{-ikx} p(x) dx = 1 - ik\mu_1 k - \mu_2 k^2/2 + o(k^2) \\ &= 1 - \sigma^2 k^2/2 + o(k^2), \quad k \rightarrow 0.\end{aligned}\tag{1}$$

- Let X_1, X_2, \dots be a sequence of iid random variables that represent the random jumps of a randomly selected particle with $\mathbb{E}[X_i] = 0$ and $\mathbb{E}[X_i^2] = \sigma^2$.
- Lévy's continuity theorem \implies the particle's location $S_n := X_1 + \dots + X_n$ satisfies

$$\begin{aligned}\mathbb{E}[e^{-ik(S_n/\sqrt{n})}] &= \prod_{j=1}^n \mathbb{E}[e^{-i(n^{-1/2}k)X_j}] = \left[1 - \frac{\sigma^2 k^2}{2n} + o\left(\frac{1}{n}\right)\right]^n \\ &\longrightarrow e^{-\frac{\sigma^2 k^2}{2}} = \int_{\mathbb{R}} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{x^2}{2\sigma^2}} e^{-ikx} dx = \mathbb{E}[e^{-ikZ}], \\ S_n/\sqrt{n} &\Rightarrow Z \sim N(0, \sigma^2), \quad \text{as } n \rightarrow \infty.\end{aligned}\tag{2}$$

- For any fixed time $t > 0$ and $c \gg 1$, the rescaled random walk

$$S_{\lfloor ct \rfloor} := X_1 + \dots + X_{\lfloor ct \rfloor} \quad (3)$$

gives the particle location at time $t > 0$ after $\lfloor ct \rfloor$ jumps.

- As the jump size is reduced by $1/\sqrt{c}$, the normalized partition location $S_{\lfloor ct \rfloor}/\sqrt{c}$ satisfies

$$\begin{aligned} \mathbb{E}[e^{-ik(S_{\lfloor ct \rfloor}/\sqrt{c})}] &= \left[1 - \frac{\sigma^2 k^2}{2c} + o\left(\frac{1}{c}\right)\right]^{\lfloor ct \rfloor} \rightarrow e^{-\frac{t\sigma^2 k^2}{2}} \\ &= \mathbb{E}[e^{-ikZ_t}] =: \hat{p}(k, t) = \frac{1}{\sqrt{2\pi\sigma^2 t}} e^{-\frac{x^2}{2\sigma^2 t}}, \end{aligned} \quad (4)$$

$$S_{\lfloor ct \rfloor}/\sqrt{c} \Rightarrow Z_t$$

by Lévy continuity theorem. Here $Z_t \sim N(0, \sigma^2 t)$ is a Brownian motion.

- Z_t can be written as an Ito type stochastic differential equation, which gives a microscopic description of diffusion (Pearson's approach)

$$dZ_t = \mu dt + \sigma dB_t. \quad (5)$$

where $\mu = 0$ and $B_t \sim N(0, t)$ is the standard Brownian motion.

- Let $\hat{p}(k, t) := e^{-\frac{t\sigma^2 k^2}{2}}$ be the FT of of the PDF $p(x, t)$, which satisfies

$$\frac{\partial \hat{p}}{\partial t} = -\frac{\sigma^2}{2} k^2 \hat{p} = \frac{\sigma^2}{2} (ik)^2 \hat{p} = \frac{\sigma^2}{2} \widehat{\frac{\partial^2 p}{\partial x^2}} \quad \longrightarrow \quad \frac{\partial p}{\partial t} = \frac{\sigma^2}{2} \frac{\partial^2 p}{\partial x^2}. \quad (6)$$

- This relates the dispersivity K to the particle jump variance σ^2 .
- The PDF satisfies a Fickian diffusion equation (as the Fokker-Planck equation of the SDE), which decays exponentially.
- The equivalence between the PDE description and the stochastic formulation also has mathematical and numerical impact
 - One can solve a diffusion PDE (the Fokker-Planck equation) to find the PDF $p(x, t)$ of the underlying stochastic process.
 - One can also use a particle tracking method to numerically solve a diffusion PDE by simulating the underlying stochastic process.

- For $\mu \neq 0$, the stochastic process $\mu t + Z_t$ satisfies the Ito SDE (5). Moreover, it has FT

$$\mathbb{E}\left[e^{-ik(\mu t + Z_t)}\right] = e^{-ik\mu t - \frac{t\sigma^2 k^2}{2}} =: \widehat{p}(k, t), \quad (7)$$

which solves

$$\frac{\partial \widehat{p}}{\partial t} = \left(-i\mu k - \frac{\sigma^2}{2} k^2\right) \widehat{p} = -\mu \frac{\partial \widehat{p}}{\partial x} + \frac{\sigma^2}{2} \frac{\partial^2 \widehat{p}}{\partial x^2}, \quad (8)$$

- which inverts to an advection-diffusion equation

$$\frac{\partial p}{\partial t} + \mu \frac{\partial p}{\partial x} - \frac{\sigma^2}{2} \frac{\partial^2 p}{\partial x^2} = 0 \quad (9)$$

as the Fokker-Plank PDE of the SDE (5).

- Derivation of the classical conservation law
 - Let $c(x, t)$ be the concentration of a solute and $q(x, t)$ be the flux. In a small cube of side δx with the cross-sectional area $A = (\delta x)^2$, the mass change δM and δc over time δt are

$$\delta M(x, t) = q(x - \delta x/2, t)A\delta t - q(x + \delta x/2, t)A\delta t = -\delta q(x, t)A\delta t,$$

$$\delta c(x, t) = \frac{\delta M(x, t)}{A\delta x} = -\frac{\delta q(x, t)\delta t}{\delta x}. \quad (10)$$

- Taking the limit as $\delta x, \delta t \rightarrow 0^+$ yields a mass conservation law

$$\frac{\delta c(x, t)}{\delta t} = -\frac{\delta q(x, t)}{\delta x} \implies \frac{\partial c}{\partial t} = -\frac{\partial q}{\partial x} \quad (11)$$

- The classical Fick's law

$$q(x, t) = -K \frac{\partial c(x, t)}{\partial x} \quad (12)$$

- assumes the particles jump locally to the left and right neighboring cells with equal probability

$$q(x, t) \approx -K \frac{\delta c(x, t)}{\delta x} = -K \frac{c(x + \delta x/2, t) - c(x - \delta x/2, t)}{\delta x}. \quad (13)$$

- The form (12) is clear for a constant K and is assumed for a variable K .
- Inserting Fick's law into (11) yields the classical Fickian diffusion PDE

$$\frac{\partial c(x, t)}{\partial t} = \frac{\partial}{\partial x} \left(K \frac{\partial c(x, t)}{\partial x} \right) = K \frac{\partial^2 c(x, t)}{\partial x^2}. \quad (14)$$

The second equal sign holds for a constant K . (14) is self-adjoint.

- Consider the Ito SDE with variable drift μ and volatility σ

$$dZ_t = \mu(t, Z_t)dt + \sigma(t, Z_t)dB_t. \quad (15)$$

- For any smooth and rapidly decaying $f(x)$, Ito's Lemma states $Y_t = f(Z_t)$ satisfies

$$dY_t = f'(Z_t)dZ_t + \frac{1}{2}f''(Z_t)dZ_t^2 = (f'(Z_t)\mu + f''(Z_t)\sigma^2/2)dt + f'(Z_t)\sigma dB_t \quad (16)$$

- Integrating (16) on any time interval $[a, b]$ gives

$$Y_b - Y_a = f(Z_b) - f(Z_a) = \int_a^b (f'(Z_t)\mu + f''(Z_t)\sigma^2/2)dt + \int_a^b f'(Z_t)\sigma dB_t. \quad (17)$$

- Taking the expectation of (17) (recall $\mathbb{E}(B_t) = 0$) yields

$$\begin{aligned} \mathbb{E}[f(Z_b) - f(Z_a)] &= \int_{\mathbb{R}} f(x)[p(x, b) - p(a, t)]dt = \int_a^b \int_{\mathbb{R}} f(x) \frac{\partial p(x, t)}{\partial t} dx dt \\ &= \int_a^b \int_{\mathbb{R}} (f'(x)\mu(x, t) + f''(x)\sigma^2(x, t)/2)p(x, t) dx dt. \end{aligned} \quad (18)$$

- Integrating the terms on the right-hand side by parts and using the fact that f is arbitrary to get the Fokker-Planck PDE

$$\frac{\partial p}{\partial t} + \frac{\partial}{\partial x} \left(\mu(x, t) p(x, t) \right) - \frac{\partial^2}{\partial x^2} \left(\frac{\sigma^2}{2} p(x, t) \right) = 0. \quad (19)$$

- For variable drift and volatility, the governing PDE is in a conservative form. Retaining conservation is of crucial importance in many applications (e.g., subsurface porous medium flow and transport, especially when the problem has high uncertainty).
- The variable σ is in the different place from that in the Fickian diffusion PDE.

- “Prehistorical development”

- Fractional calculus stemmed from a question by L'Hopital (1695) to Leibniz on the meaning of $\frac{d^n y}{dx^n}$ for $n = 1/2$. Leibniz's reply (Sept 30 1695): "... This is an apparent paradox from which, one day, useful consequences will be drawn. ..."
- Euler observed that the differentiation formula

$$\frac{d^n x^\alpha}{dx^n} = \alpha(\alpha - 1) \cdots (\alpha - n + 1)x^{\alpha-n} = \frac{\Gamma(\alpha + 1)}{\Gamma(\alpha - n + 1)}x^{\alpha-n}$$

has a meaning for non-integer n (1738).

- Laplace proposed the idea of non-integer order differentiation by means of an integral (1812).
- Fourier suggested some integral representation of fractional differentiation (1822).

- Fractional calculus really began with Abel and Liouville
 - Abel solved the integral equation (1823)

$$\int_a^x \phi(t)(x-t)^{-\mu} dt = f(x), \quad x > a, \quad 0 < \mu < 1$$

- Liouville made the major contribution to the theory (1832-1837)

$$D^\alpha f(x) = \sum_{k=0}^{\infty} c_k a_k^\alpha e^{a_k x}, \quad \text{for } f(x) = \sum_{k=0}^{\infty} c_k e^{a_k x}.$$

He proposed $D^\alpha f(x) := \lim_{h \rightarrow 0} \frac{(\Delta_h^\alpha f)(x)}{h^\alpha}$ but didn't pursue it.

- Riemann came up with today's fractional integration formula in 1847 (when still a student, but published in 1876 ten years after his death).
- Grünwald (1867) and Letnikov (1868) introduced the definition

$$D^\alpha f(x) := \lim_{h \rightarrow 0} \frac{(\Delta_h^\alpha f)(x)}{h^\alpha}.$$

Letnikov proved that this definition coincides with Riemann's.

- For any $n \in \mathbb{N}$, the iterated integrals can be expressed by

$$\begin{aligned}
 {}_a I_x^1 f(x) &:= \int_a^x f(y) dy, & {}_a I_x^2 f(x) &:= \int_a^x ({}_a I_z^1 f)(z) dz \\
 &= \int_a^x \int_a^z f(y) dy dz = \int_a^x \int_y^x f(y) dz dy = \int_a^x (x-y) f(y) dy, \dots \\
 {}_a I_x^n f(x) &:= \int_a^x ({}_a I_z^{n-1} f)(z) dz = \int_a^x \int_a^z \frac{(z-y)^{n-2}}{(n-2)!} f(y) dy dz \\
 &= \int_a^x \int_y^x \frac{(z-y)^{n-2}}{(n-2)!} f(y) dz dy = \frac{1}{\Gamma(n)} \int_a^x (x-y)^{n-1} f(y) dy.
 \end{aligned}$$

Here the Gamma function $\Gamma(\beta) := \int_0^\infty e^{-t} t^{\beta-1} dt$ and $\Gamma(n) = (n-1)!$.

- For any $\beta \in \mathbb{R}^+$, define the left and right fractional integrals as

$$\begin{aligned}
 {}_a I_x^\beta f(x) &:= \frac{1}{\Gamma(\beta)} \int_a^x (x-y)^{\beta-1} f(y) dy, \\
 {}_x I_b^\beta f(x) &:= \frac{1}{\Gamma(\beta)} \int_x^b (y-x)^{\beta-1} f(y) dy.
 \end{aligned} \tag{20}$$

- The Riemann-Liouville fractional derivatives of order $\alpha = n - \beta$, $0 < \beta < 1$

$$\begin{aligned} {}_a^{RL}D_x^\alpha f(x) &:= D^n {}_aI_x^\beta f(x) = \frac{1}{\Gamma(\beta)} \frac{d^n}{dx^n} \int_a^x (x-y)^{\beta-1} f(y) dy, \\ {}_x^{RL}D_b^\alpha f(x) &:= (-1)^n D^n {}_xI_b^\beta f(x) = \frac{(-1)^n}{\Gamma(\beta)} \frac{d^n}{dx^n} \int_x^b (y-x)^{\beta-1} f(y) dy. \end{aligned} \quad (21)$$

- The Caputo fractional derivatives of order $\alpha = n - \beta$, $0 < \beta < 1$

$$\begin{aligned} {}_a^C D_x^\alpha f(x) &:= {}_aI_x^\beta D^n f(x) = \frac{1}{\Gamma(\beta)} \int_a^x (x-y)^{\beta-1} f^{(n)}(y) dy, \\ {}_x^C D_b^\alpha f(x) &:= (-1)^n {}_xI_b^\beta D^n f(x) = \frac{(-1)^n}{\Gamma(\beta)} \int_x^b (y-x)^{\beta-1} f^{(n)}(y) dy. \end{aligned} \quad (22)$$

- Fractional derivatives defined via Fourier transform

$$-\infty D_x^\alpha f(x) := \mathcal{F}^{-1}[(ik)^\alpha \hat{f}(k)], \quad x D_\infty^\alpha f(x) := \mathcal{F}^{-1}[(-ik)^\alpha \hat{f}(k)]. \quad (23)$$

- Integer-order derivatives can be expressed as limit of difference quotients

$$\begin{aligned}
 f'(x) &= \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} (I - B_\varepsilon) f(x) = \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} [f(x) - f(x - \varepsilon)] \\
 f^{(n)}(x) &= \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon^n} (I - B_\varepsilon)^n f(x) = \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon^n} \sum_{k=0}^n g_k^{(n)} f(x - k\varepsilon).
 \end{aligned} \tag{24}$$

with $g_k^{(n)} := (-1)^k \binom{n}{k}$ being the binomial coefficients.

- The n in ε^n and $\binom{n}{k}$ in (24) counts for the order of the derivative.
- The n in $\sum_{k=0}^n$ in (24) counts for the number of summands.
- If we replace n in the former by α and n in the latter by the number of summands to the left boundary $x = a$, we obtain the definition of the Grünwald-Letnikov fractional derivatives of order α

$$\begin{aligned}
 {}_a^{GL} D_x^\alpha f(x) &:= \lim_{\varepsilon \rightarrow 0^+} \frac{1}{\varepsilon^\alpha} \sum_{k=0}^{\lfloor (x-a)/\varepsilon \rfloor} g_k^{(\alpha)} f(x - k\varepsilon), \\
 {}_x^{GL} D_b^\alpha f(x) &:= \lim_{\varepsilon \rightarrow 0^+} \frac{(-1)^{\lceil \alpha \rceil}}{\varepsilon^\alpha} \sum_{k=0}^{\lfloor (b-x)/\varepsilon \rfloor} g_k^{(\alpha)} f(x + k\varepsilon).
 \end{aligned} \tag{25}$$

- Under appropriate smoothness assumptions, the Riemann-Liouville fractional derivatives and Grünwald-Letnikov fractional derivatives coincide

$${}^GL D_x^\alpha f(x) = {}^{RL} D_x^\alpha f(x), \quad {}^GL D_b^\alpha f(x) = {}^{RL} D_b^\alpha f(x). \quad (26)$$

- The Riemann-Liouville fractional derivatives and the Caputo fractional derivatives differ by singular boundary terms. For example, for $0 < \alpha < 1$,

$${}_0^C D_x^\alpha f(x) = {}^{RL} D_x^\alpha f(x) - \frac{f(0)x^{-\alpha}}{\Gamma(1-\alpha)}. \quad (27)$$

- All the three fractional derivatives (with $a = -\infty$ and $b = \infty$) coincide for rapidly decaying f on \mathbb{R} and equal to those defined by Fourier transforms (Multidimensional cases much subtle).

- Example: Let $f(x) = 1$ for $x > 0$. Then for $0 < \alpha < 1$, ${}^C_0 D_x^\alpha f(x) = 0$ but

$$\begin{aligned} {}^{RL}_0 D_x^\alpha f(x) &:= D_0 I_x^{1-\alpha} f(x) = \frac{1}{\Gamma(1-\alpha)} \frac{d}{dx} \int_0^x (x-y)^{-\alpha} dy \\ &= \frac{d}{dx} \frac{x^{1-\alpha}}{\Gamma(2-\alpha)} = \frac{x^{-\alpha}}{\Gamma(1-\alpha)} \neq 0. \end{aligned} \quad (28)$$

This is consistent with (27).

- Let $\tilde{f}(s) \equiv \mathcal{L}[f](s) := \int_0^\infty e^{-st} f(t) dt$ be the LT of f . It is shown that

$$\mathcal{L}[{}^C_0 D_t^\alpha f(t)] = s^\alpha \tilde{f}(s) - s^{\alpha-1} f(0), \quad \mathcal{L}[{}^{RL}_0 D_t^\alpha f(t)] = s^\alpha \tilde{f}(s), \quad 0 < \alpha < 1. \quad (29)$$

$\mathcal{L}[{}^C_0 D_t^\alpha f(t)]$ resembles that of f' , and has been used in time FPDE.

- It was found that the dispersive transport of electrons in operation of photocopiers and laser printers could not be modeled properly by the classical Fickian diffusion PDE (Scher & Montroll 1975).
 - Charges moving in media get trapped by local imperfections and then get released due to thermal fluctuations.
- In groundwater contaminant transport, remediation is not so effective as predicted by the integer-order advection-diffusion PDEs
 - The contaminant in groundwater gets trapped to low permeability zone and gets released when the contaminant is cleaned.
- Einstein and Pearson's assumptions are violated in these processes
 - These assumptions hold for homogeneous medium,
 - but fail for heterogeneous medium.

- The current modeling of transport process in heterogeneous media is
 - to use integer-order PDEs (valid for homogeneous medium),
 - to tweak free parameters that multiply pre-set integer-order PDEs.
- Field tests show that
 - contaminant plumes often exhibit a power-law decaying tail in heterogeneous media,
 - integer-order PDE model, characterized by an exponentially decaying tail, struggles a variable coefficient fit (of the data at each location),
 - FPDE model, characterized by a power-law decaying tail, can fit all the data with a constant coefficient.
- Many anomalous diffusion processes were found in various disciplines
 - signaling of biological cells, anomalous electrodiffusion in nerve cells
 - foraging behavior of animals, electrochemistry, physics, finance
 - fluid and continuum mechanics, viscoelastic and viscoplastic flow

- A fractional Fick's law assumes that the underlying particles have global jumps, i.e., $\delta c(x, t)$ is increased by an amount of $g_k^{(\alpha-1)} c(x - k\delta x, t)$, i.e.,

$$q(x, t) = -K \frac{\partial^{\alpha-1} c(x, t)}{\partial x^{\alpha-1}}, \quad 1 < \alpha < 2. \quad (30)$$

Here the fractional derivatives are Grünwald-Letnikov type. Since $g_k^{(\alpha-1)}$ decay like $O(k^{-\alpha})$, the particle jumps have a heavy tail.

- Inserting (30) into (11) yields a space FPDE

$$\frac{\partial c}{\partial t} = -\frac{\partial q}{\partial x} = \frac{\partial}{\partial x} \left(K \frac{\partial^{\alpha-1} c(x, t)}{\partial x^{\alpha-1}} \right) = K \frac{\partial^\alpha c(x, t)}{\partial x^\alpha}. \quad (31)$$

The second equal sign holds for a constant K .

- In anomalous diffusion a particle's motion may have very different waiting times/jump sizes. Classical random walk does not apply.
 - Let X_1, X_2, \dots be a sequence of iid random jumps of a particle with $\mathbb{E}[X_i] = 0$ and $\mathbb{P}[X > x] = Cx^{-\alpha}$ where $C > 0$ and $1 < \alpha < 2$.
 - $\mathbb{E}[X^p] = \alpha/(\alpha - p)$ for $0 < p < \alpha$ or ∞ for $p \geq \alpha$. Central limit theorem (Fickian diffusion or SDE by Brownian motion) fails to apply.
 - The FT of a different scaling of $S_{[ct]}$ yields

$$\mathbb{E}[e^{-ikc^{-1/\alpha}S_{[ct]}}] = \left[1 + \frac{(ik)^\alpha}{c} + O(c^{-2/\alpha})\right]^{[ct]} \rightarrow e^{t(ik)^\alpha}. \quad (32)$$

- Lévy's continuity theorem concludes that a properly scaled $S_{[ct]}$ converges to an α stable Lévy process Z_t

$$e^{t(ik)^\alpha} = \mathbb{E}[e^{-ikZ_t}] = \hat{p}(k, t) = \int_{\mathbb{R}} e^{-ikx} p(x, t) dx, \quad (33)$$

i.e., $c^{-1/\alpha}S_{[ct]} \Rightarrow Z_t$.

- Unlike Gaussian case, there is no analytical expression for $p(x, t)$ now.

- The Pearson's viewpoint gives rise to an SDE driven by an Lévy process

$$dX_t = \mu dt + \sigma dL_t. \quad (34)$$

- Einstein's approach: Note that $\hat{p}(k, t) = e^{t(ik)^\alpha}$ solves

$$\frac{d\hat{p}}{dt} = (ik)^\alpha \hat{p} = \frac{\widehat{\partial^\alpha p}}{\partial x^\alpha} \quad (35)$$

- which inverts to

$$\frac{\partial p}{\partial t} = \frac{\partial^\alpha p}{\partial x^\alpha}. \quad (36)$$

- The PDF of finding a particle somewhere in space satisfies a (space-fractional) PDE, which decays algebraically $O(x^{-(\alpha+1)})$.
- This justifies why FPDEs model transport processes exhibiting anomalous diffusion, long-range time memory or space interactions more accurately than classical integer-order PDEs.

*Thank You
for Your Attention!*