



Model reduction, data-based and advanced discretization in computational mechanics

On the physical interpretation of fractional diffusion

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ABSTRACT

Even if the diffusion equation has been widely used in physics and engineering, and its physical content is well understood, some variants of it escape fully physical understanding. In particular, anomalous diffusion appears in the so-called fractional diffusion equation, whose main particularity is its non-local behavior, whose physical interpretation represents the main part of the present work.

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1. Introduction

1.1. From standard diffusion to anomalous diffusion

The microscopic nature of diffusion is evident from the pioneering works of Einstein, who considered the increment in the particle position Δ (assumed defined, for the sake of simplicity, in the unbounded one-dimensional axis x) as a random variable, with a probability density given by $\phi(\Delta)$. Thus, the particles balance can be expressed by both

$$\rho(x, t + \tau) = \rho(x, t) + \frac{\partial \rho}{\partial t} \tau + \Theta(\tau^2) \quad (1)$$

and

$$\rho(x, t + \tau) = \int_{\mathbb{R}} \rho(x + \Delta, t) \phi(\Delta) d\Delta \quad (2)$$

Developing $\rho(x + \Delta, t)$,

$$\rho(x + \Delta, t) = \rho(x, t) + \frac{\partial \rho}{\partial x} \Delta + \frac{1}{2} \frac{\partial^2 \rho}{\partial x^2} \Delta^2 + \Theta(\Delta^3) \quad (3)$$

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which, substituted into the right-hand side of Eq. (1), and taking into account the normality and expected symmetry

$$\begin{cases} \int_{\mathbb{R}} \phi(\Delta) d\Delta = 1 \\ \int_{\mathbb{R}} \Delta \phi(\Delta) d\Delta = 0 \end{cases} \tag{4}$$

leads, after equating Eqs. (1) and (2), to

$$\rho(x, t) + \frac{\partial \rho}{\partial t} \tau = \rho(x, t) + \frac{1}{2} \frac{\partial^2 \rho}{\partial x^2} \int_{\mathbb{R}} \Delta^2 \phi(\Delta) d\Delta \tag{5}$$

or

$$\frac{\partial \rho}{\partial t} \tau = \frac{1}{2} \frac{\partial^2 \rho}{\partial x^2} \int_{\mathbb{R}} \Delta^2 \phi(\Delta) d\Delta \tag{6}$$

If we define the diffusion coefficient D as

$$D = \frac{1}{2\tau} \int_{\mathbb{R}} \Delta^2 \phi(\Delta) d\Delta \tag{7}$$

the particle balance, also known as the diffusion equation, is given by

$$\frac{\partial \rho}{\partial t} = D \frac{\partial^2 \rho}{\partial x^2} \tag{8}$$

The integration of this equation, assuming that all the particles are localized at the origin at the initial time, $\rho(x, t = 0) = \delta(x)$, leads to

$$\rho(x, t) = \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}} \tag{9}$$

whose second-order moment (variance) scales with time

$$\langle x^2 \rangle = 2Dt \tag{10}$$

that is, the mean squared displacement scales with the elapsed time t , and the diffusion coefficient D .

The same equation can be derived by describing diffusion as a random walk. Again, for the sake of simplicity, we restrict our discussion to the 1D case, with the x -axis equipped with a grid of size Δx . In a discrete time step Δt , the test particle is assumed to jump to one of its nearest neighbor sites, with random direction. Such a process can be modeled by the master equation that writes, at site j ,

$$W_j(t + \Delta t) = \frac{1}{2} W_{j+1}(t) + \frac{1}{2} W_{j-1}(t) \tag{11}$$

where $W_j(t)$ represents the probability of having the particle at site j at time t and the pre-factor $1/2$ accounts for the direction isotropy of the jumps.

By taking classical Taylor expansions,

$$\begin{cases} W_j(t + \Delta t) = W_j(t) + \left. \frac{\partial W_j(t)}{\partial t} \right|_t \Delta t + \Theta(\Delta t^2) \\ W_{j+1}(t) = W_j(t) + \left. \frac{\partial W(t)}{\partial x} \right|_j \Delta x + \frac{1}{2} \left. \frac{\partial^2 W(t)}{\partial x^2} \right|_j \Delta x^2 + \Theta(\Delta x^3) \\ W_{j-1}(t) = W_j(t) - \left. \frac{\partial W(t)}{\partial x} \right|_j \Delta x + \frac{1}{2} \left. \frac{\partial^2 W(t)}{\partial x^2} \right|_j \Delta x^2 - \Theta(\Delta x^3) \end{cases} \tag{12}$$

that, injected into Eq. (11), yield

$$\frac{\partial W}{\partial t} = D \frac{\partial^2 W}{\partial x^2} \tag{13}$$

with D defined in the limit of $\Delta x \rightarrow 0$ and $\Delta t \rightarrow 0$ by

$$D = \frac{\Delta x^2}{2\Delta t} \tag{14}$$

which leads to the diffusion equation previously derived.

In complex fluids, micro-rheological experiments often exhibit anomalous sub-diffusion or sticky diffusion, in which the mean square displacement of Brownian tracer particles is found to scale as $\langle x^2 \rangle \propto t^\alpha$, $0 < \alpha < 1$ (see [1] and the

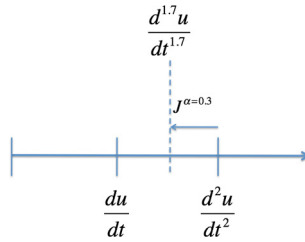


Fig. 1. Schematic cartoon of the derivative of order 1.7.

references therein). In these cases, the use of non-integer derivatives can constitute an appealing alternative, as it allows one to correctly reproduce the observed physical behavior while keeping the model as simple as possible. Moreover, from a physical point of view, the use of non-integer derivatives introduces a degree of non-locality that seems to be in agreement with the intrinsic nature of the physical system, as discussed later.

As proved in [2,3] fractional diffusion models can be derived from continuous time random walks – CTRW – leading to a fractional diffusion equation in the same manner as standard random walks lead to the usual diffusion equation, where subdiffusion is associated with long rest, whereas superdiffusion is related with long jumps. A detailed derivation can be found in [4].

In [5], we reinterpreted, by using fractional diffusion, the rheological findings reported in [6], which were difficult to explain using standard models. However, that purely phenomenological route, which assumed non-standard randomizing mechanisms, failed to give a physical picture of the subjacent reality. Thus, despite the fact that a surprising excellent agreement between the predictions and the experimental measurements, both in linear viscoelasticity and relaxation after a step strain, was found, no physical mechanisms were proposed to justify the considered anomalous diffusion.

A physically-based explanation was advanced in [7] where particles involved in the suspension were subjected to the bombardment coming from the neighbor molecules of solvent, a viscous drag and an elastic term related to the interaction with neighboring particles. The stochastic inertia-free simulation proved that the mean square displacement does not scale with the time, but with a power of it, lower than one. The analysis of the covariance reveals that the motion can be assimilated to a fractional Brownian motion, that allowed us to associate such a motion with the solution to a fractional Fokker–Planck diffusion equation.

Other anomalies have been reported and explained through involving fractional models. One of them concerns the fact that the apparent conductivity in almost one-dimensional systems (e.g., carbon nanotubes) or two-dimensional (e.g., graphene) depends on the systems size, being this dependence more intense when the system dimensionality decreases [8]. These works claimed the need of associating fractional models with fractal media [9,10].

1.2. Fractional derivatives

In this section, we propose a general diffusive flux definition based on the use of fractional derivatives. This fractional flux will be coupled with the usual balance equation (which we assume of integer nature). Before making these proposals and developments, we start by revisiting some key results of fractional calculus considered all along the present work.

There exist many good books on fractional calculus and fractional differential equations (e.g., [11,12]). We summarize here the main concepts needed to understand the developments carried out below.

We start with the formula attributed to Cauchy to evaluate the n -th integration, $n \in \mathbb{N}$, of a function $f(t)$:

$$J^n f(t) := \int \dots \int f(\tau) d\tau = \frac{1}{(n-1)!} \int_0^t (t-\tau)^{n-1} f(\tau) d\tau \tag{15}$$

This can be rewritten as

$$J^n f(t) = \frac{1}{\Gamma(n)} \int_0^t (t-\tau)^{n-1} f(\tau) d\tau \tag{16}$$

where $\Gamma(n) = (n-1)!$ is the gamma function. The latter being, in fact, defined for any real value $\alpha \in \mathbb{R}$, we can define the fractional integral from

$$J^\alpha f(t) := \frac{1}{\Gamma(\alpha)} \int_0^t (t-\tau)^{\alpha-1} f(\tau) d\tau \tag{17}$$

If we consider the fractional derivative of order α and select an integer $m \in \mathbb{N}$ such that $m-1 < \alpha < m$, then it suffices to consider an integer m -order derivative combined with a $(m-\alpha)$ fractional integral (this is depicted in sketch form in Fig. 1).

Obviously, we could take the derivative of the integral or the integral of the derivative, resulting in the Riemann–Liouville and Caputo definitions of the fractional derivative usually denoted by $D^\alpha f(t)$ and $D_*^\alpha f(t)$, respectively,

$$D^\alpha f(t) = \begin{cases} \frac{d^m}{dt^m} \left(\frac{1}{\Gamma(m-\alpha)} \int_0^t \frac{f(\tau)}{(t-\tau)^{\alpha+1-m}} d\tau \right), & m-1 < \alpha < m \\ \frac{d^m f(t)}{dt^m}, & \alpha = m \end{cases} \quad (18)$$

and

$$D_*^\alpha f(t) = \begin{cases} \frac{1}{\Gamma(m-\alpha)} \left(\int_0^t \frac{\frac{d^m f(\tau)}{d\tau^m}}{(t-\tau)^{\alpha+1-m}} d\tau \right), & m-1 < \alpha < m \\ \frac{d^m f(t)}{dt^m}, & \alpha = m \end{cases} \quad (19)$$

Because these approaches to the fractional derivative began with an expression for the repeated integration of a function, one could consider a similar approach for the derivative. This was the route considered by Grunwald and Letnikov (GL) defining the so-called “differintegral”, which leads to the fractional counterpart of the usual finite differences.

When considering space differential operators, the left- and right-hand-side forms of the Riemann–Liouville and Caputo definitions are used [13]. Thus we consider the definitions of both derivatives

$${}_0^x D^\alpha f(x) = \frac{d^m}{dx^m} \left(\frac{1}{\Gamma(m-\alpha)} \int_0^x \frac{f(\xi)}{(x-\xi)^{\alpha+1-m}} d\xi \right) \quad (20)$$

and

$${}_x^L D^\alpha f(x) = \frac{d^m}{dx^m} \left(\frac{1}{\Gamma(m-\alpha)} \int_x^L \frac{f(\xi)}{(\xi-x)^{\alpha+1-m}} d\xi \right) \quad (21)$$

in the case of the Riemann–Liouville, and

$${}_0^x D_*^\alpha f(x) = \frac{1}{\Gamma(m-\alpha)} \left(\int_0^x \frac{\frac{d^m f(\xi)}{d\xi^m}}{(x-\xi)^{\alpha+1-m}} d\xi \right) \quad (22)$$

and

$${}_x^L D_*^\alpha f(x) = \frac{1}{\Gamma(m-\alpha)} \left(\int_x^L \frac{\frac{d^m f(\xi)}{d\xi^m}}{(\xi-x)^{\alpha+1-m}} d\xi \right) \quad (23)$$

when considering the Caputo fractional derivative.

One important property that will be used all along this work is the fact that, when the derivative approaches an integer value, the associated expression reduces to its standard integer expression. For the sake of completeness, we reproduce the proof it in the case of the Riemann–Liouville derivative. For that purpose, we consider

$${}_a^t D^\alpha f(t) = \frac{d^m}{dt^m} \left(\frac{1}{\Gamma(m-\alpha)} \int_a^t \frac{f(\tau)}{(t-\tau)^{\alpha+1-m}} d\tau \right) \quad (24)$$

that, by integrating by parts, results

$${}_a^t D^\alpha f(t) = \frac{d^m}{dt^m} \left(\frac{(t-a)^{m-\alpha} f(a)}{\Gamma(m-\alpha+1)} + \frac{1}{\Gamma(m-\alpha+1)} \int_a^t (t-\tau)^{m-\alpha} \frac{df(\tau)}{d\tau} d\tau \right) \quad (25)$$

By taking the limit when $\alpha \rightarrow m$ leads to

$${}_a^t D^{\alpha \rightarrow m} f(t) = \frac{d^m}{dt^m} (f(a) + (f(t) - f(a))) = \frac{d^m f(t)}{dt^m} \quad (26)$$

where, other than the interest of proving that fractional derivatives approach with continuity the ones of integer order, we just proved that, for any function $f(t)$, when $\alpha \rightarrow m$

$$\text{Lim}_{\alpha \rightarrow m} \frac{1}{\Gamma(m-\alpha)} \int_a^t (t-\tau)^{m-\alpha-1} f(\tau) d\tau = f(t) \quad (27)$$

1.3. Paper outline

The approach based on the use of CTRW remains too microscopic to allow a simple and physical interpretation of the resulting macroscopic fractional equations. In this paper, we focus in superdiffusion and we are following two different routes to extract its physical content, based on the use of the Riemann–Liouville and Caputo fractional derivatives. Next section defines fractional fluxes, the associated fractional diffusion equation, and illustrates the main implications on a simple numerical case. Then, Section 3 proposes a physical view of the Riemann–Liouville – RL – fractional diffusion, while Section 4 addresses a similar analysis on the Caputo fractional diffusion, to conclude with a short discussion on the proposed physical interpretations.

2. From fractional fluxes to the fractional diffusion equation

The Fourier or Fick equation for standard diffusion writes

$$Q(x) = -\mathbb{K} \frac{du(x)}{dx} \tag{28}$$

where \mathbb{K} is the diffusion coefficient.

This equation can be generalized, for non-integer derivatives, in the following way

$$Q^\alpha(x) = -\frac{1}{2}\mathbb{K} \left({}_0^x D^\alpha u(x) + {}_x^L D^\alpha u(x) \right) \tag{29}$$

and

$$Q_*^\alpha(x) = -\frac{1}{2}\mathbb{K} \left({}_0^x D_*^\alpha u(x) + {}_x^L D_*^\alpha u(x) \right) \tag{30}$$

for the Riemann–Liouville and Caputo derivatives respectively; it can be noticed that the spatial gradient operator has been symmetrized to represent the symmetric (spatial) physics of diffusion.

The fractional diffusion equation results from the mass or energy balances,

$$\frac{\partial u}{\partial t} = \frac{d}{dx} F(x) \tag{31}$$

where $F(x)$ refers to the flux at position $x \in (0, L) \subset \mathbb{R}$, in particular the standard or anomalous fluxes, $Q(x)$, $Q^\alpha(x)$ or $Q_*^\alpha(x)$.

In what follows, we restrict our analysis to the case where $m = 1$ and $0 < \alpha \leq m = 1$.

2.1. Numerical results

To compare the heat flux behavior in the case of standard and fractional fluxes, we solve the heat equation in the domain $(0, L)$, for $L = 1$ and $L = 5$, while enforcing as boundary conditions $u(x = 0) = 0$ and $u(x = L) = L$, with conductivity $\mathbb{K} = 1$, $\alpha = 1$ and $\alpha = 0.5$ in the standard and fractional flux, respectively.

In the standard case, the solution becomes $u(x) = x$, and consequently the associated flux $u'(x) = 1$. In the fractional case (when using the Caputo fractional derivative), the expected solution is again $u(x) = x$, however fluxes are expected to depend on the domain's length. Figs. 2 and 3 corroborate these expectations.

3. Riemann–Liouville – RL – fractional diffusion

When considering the RL flux Q^α , the left contribution to the flux involves the integral

$${}_0^x D^\alpha u(x) = \frac{d}{dx} \left(\frac{1}{\Gamma(1 - \alpha)} \int_0^x \frac{u(\xi)}{(x - \xi)^\alpha} d\xi \right) \tag{32}$$

We just proved that when $\alpha \rightarrow 1$, it becomes ${}_0^x D^{\alpha \rightarrow 1} u(x) = \frac{du(x)}{dx}$, that is, the standard integer derivative, leading to the standard diffusive flux. However, the previous equation reflects the fact that, for any choice of α , real or integer, the flux can be viewed as the result of an integral, even if, in the integer case, the integral collapses to the local gradient (in any case an alternative integral form can be associated with it).

To better apprehend its physical content, we proceed by taking its derivative [14], and even if the derivative will be introduced into the integral, the resulting expression will differ from the Caputo formulation, as proved later.

By applying the Leibniz's rule to the right-hand member of Eq. (32), it results (after taking into account that, as proved in [14], the term at x cancels with the right-flux contribution)

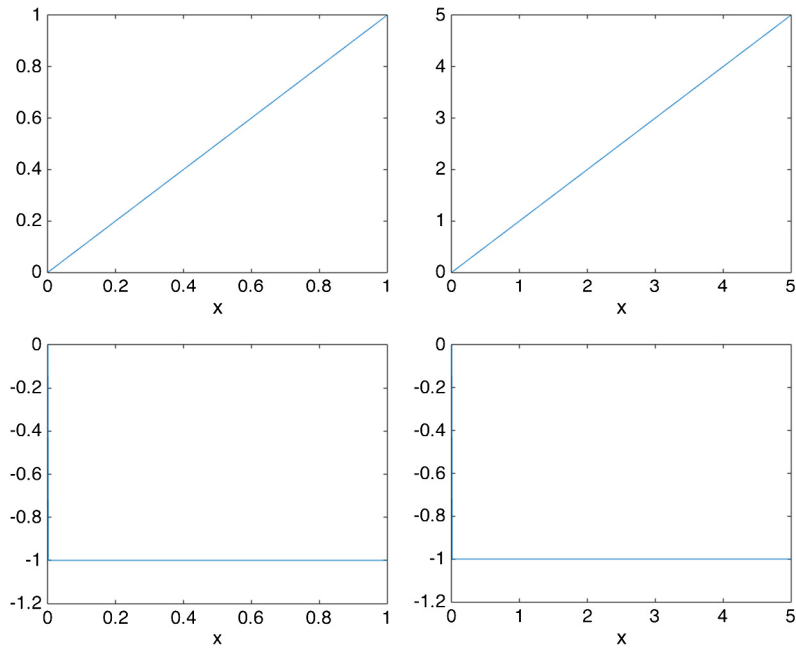


Fig. 2. Standard flux model with $\kappa = 1$: (top) temperature field; (bottom) flux field; (left) $L = 1$ and (right) $L = 5$.

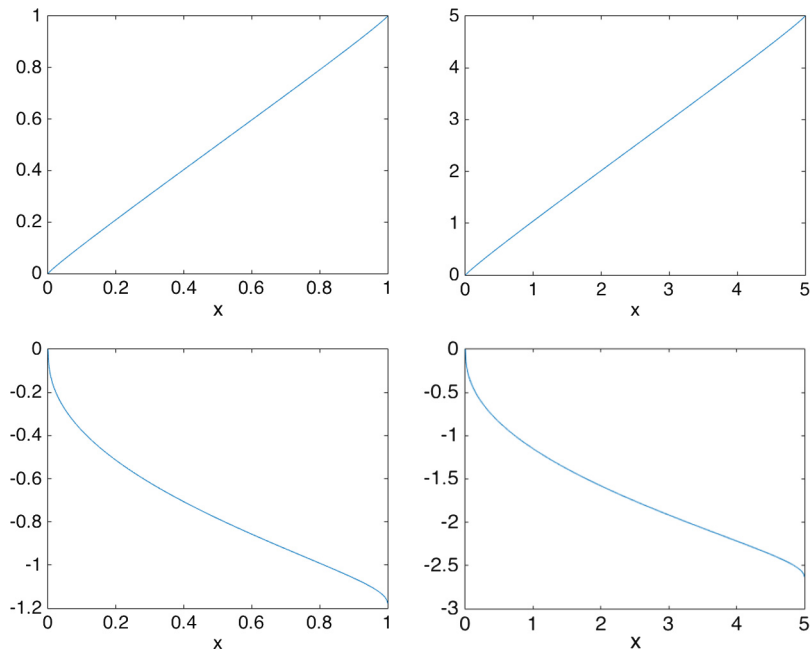


Fig. 3. Fractional flux model with $\kappa = 1$ and $\alpha = 0.5$: (top) temperature field; (bottom) flux field; (left) $L = 1$ and (right) $L = 5$.

$$\frac{d}{dx} \left(\frac{1}{\Gamma(1-\alpha)} \int_0^x \frac{u(\xi)}{(x-\xi)^\alpha} d\xi \right) = -\frac{\alpha}{\Gamma(1-\alpha)} \int_0^x \frac{1}{(x-\xi)^{\alpha+1}} u(\xi) d\xi \tag{33}$$

where the derivative applies on the kernel without affecting the field $u(\xi)$, making the difference with respect to the Caputo's expression addressed later.

Thus, the resulting flux at position x , $Q^\alpha(x)$, reads

$$Q^\alpha(x) = \frac{1}{2}K \frac{\alpha}{\Gamma(1-\alpha)} \left\{ \int_0^x \frac{1}{(x-\xi)^{\alpha+1}} u(\xi) d\xi - \int_x^L \frac{1}{(\xi-x)^{\alpha+1}} u(\xi) d\xi \right\} \tag{34}$$

This expression reflects the fact that the field $u(\xi)$ at position ξ induces a flux at x , independently of the distance between ξ and x , even if, as expected, the weight affecting the contribution of $u(\xi)$ on the flux at x decreases with the mutual distance, in particular with $|x-\xi|^{1+\alpha}$. This result is not totally surprising, because it seems in agreement with the Einstein rationale exposed in the *Introduction* or its extended CTRW formulation [4]. In that approach, there is a non-zero probability that a particle located far from x reaches x in a single time step.

If we consider, in Eq. (34), both integrals for the limit case $\alpha \approx 1$ and assume that the main contribution to both integrals occurs in the interval $[x-\epsilon/2, x+\epsilon/2]$, it results

$$\begin{aligned} \int_0^x \frac{1}{(x-\xi)^2} u(\xi) d\xi - \int_x^L \frac{1}{(\xi-x)^2} u(\xi) d\xi &\approx \int_{x-\epsilon/2}^x \frac{1}{(x-\xi)^2} u(\xi) d\xi - \int_x^{x+\epsilon/2} \frac{1}{(\xi-x)^2} u(\xi) d\xi \\ &\approx \frac{1}{(\frac{\epsilon}{2})^2} u\left(x-\frac{\epsilon}{2}\right) \frac{\epsilon}{2} - \frac{1}{(\frac{\epsilon}{2})^2} u\left(x+\frac{\epsilon}{2}\right) \frac{\epsilon}{2} = \frac{2}{\epsilon} \left(u\left(x-\frac{\epsilon}{2}\right) - u\left(x+\frac{\epsilon}{2}\right) \right) \end{aligned} \tag{35}$$

Now, by expressing

$$u\left(x-\frac{\epsilon}{2}\right) = \frac{u(x-\epsilon) + u(x)}{2} \tag{36}$$

and

$$u\left(x+\frac{\epsilon}{2}\right) = \frac{u(x+\epsilon) + u(x)}{2} \tag{37}$$

introducing both into Eq. (35) leads to

$$\frac{2}{\epsilon} \left(u\left(x-\frac{\epsilon}{2}\right) - u\left(x+\frac{\epsilon}{2}\right) \right) = \frac{u(x-\epsilon) - u(x+\epsilon)}{\epsilon} \approx -2 \frac{du(x)}{dx} \tag{38}$$

which, as expected, is related to the usual gradient with the opposite sign, which combined with Eq. (34), results in the standard flux. The main difference with fractional diffusion is that, when α differs from one, the integral requires richer approximation involving larger intervals around x .

An immediate consequence is that, if the field $u(x)$ is symmetric with respect to x , the net flux vanishes. Another important consequence is that the physics induces a characteristic length, the one characterizing the domain around x , whose contribution to the integral can not be ignored. When α decreases, this characteristic length increases, and then transport properties will depend on the domain size L , a fact which could explain the findings reported in [15,16]. When $\alpha \approx 0$, the integrals involved in Eq. (34) diverge.

To apply now the space derivative involved in the balance equation (31), it suffices to consider the derivative of Eq. (34) using again the Leibniz rule, which implies the second derivative of the kernel function.

Thus, the main consequence of using the Riemann–Liouville derivative is the obtention of a non-local integral form implying that the far field (far with respect to x) affects the flux at position x , in agreement with the microscopic interpretation of diffusion from continuous time random walk, and more particularly its Levy variant. The case of standard diffusion is not an exception; it can be formulated and interpreted within the same framework, even if its final description becomes local.

4. Caputo fractional diffusion

Now, we perform a similar analysis, but now considering the Caputo fractional derivative. The flux in this case writes

$$Q_*^\alpha = -\frac{1}{2}K \left({}_0^x D_*^\alpha u(x) + {}_x^L D_*^\alpha u(x) \right) \tag{39}$$

with

$${}_0^x D_*^\alpha u(x) = \frac{1}{\Gamma(1-\alpha)} \left(\int_0^x \frac{1}{(x-\xi)^\alpha} \frac{du(\xi)}{d\xi} d\xi \right) \tag{40}$$

It is important to note that, by using the previous results, integral (40) results in

$${}_0^x D_*^{\alpha \rightarrow 1} u(x) = \frac{du(x)}{dx} \tag{41}$$

but it is important to highlight its physical integral nature.

Thus, the net flux $Q_*^\alpha(x)$ reads

$$Q_*^\alpha(x) = -\frac{1}{2}K \frac{1}{\Gamma(1-\alpha)} \left\{ \int_0^x \frac{1}{(x-\xi)^\alpha} \frac{du(\xi)}{d\xi} d\xi + \int_x^L \frac{1}{(\xi-x)^\alpha} \frac{du(\xi)}{d\xi} d\xi \right\} \tag{42}$$

This expression states that the flux at position x depends on the existing field first-order derivative at position ξ with an undoubtable physical content, expressing the flux from the derivatives at different length scales, as discussed later.

The point in which the Caputo route seems advantageous from a conceptual viewpoint concerns its application on the balance equation that, making use of the fractional derivatives composition rule, reads

$$\frac{d}{dx} Q_*^\alpha(x) = -\frac{1}{2}K \left({}_0^x D_*^{\alpha+1} u(x) + {}_x^L D_*^{\alpha+1} u(x) \right) \tag{43}$$

or

$$\frac{d}{dx} Q_*^\alpha(x) \propto \left\{ \int_0^x \frac{1}{(x-\xi)^\alpha} \frac{d^2 u(\xi)}{d\xi^2} d\xi + \int_x^L \frac{1}{(\xi-x)^\alpha} \frac{d^2 u(\xi)}{d\xi^2} d\xi \right\} \tag{44}$$

When $\alpha \rightarrow 1$, by using the previous results,

$$\lim_{\alpha \rightarrow 1} \frac{1}{\Gamma(1-\alpha)} \left\{ \int_0^x \frac{1}{(x-\xi)^\alpha} \frac{d^2 u(\xi)}{d\xi^2} d\xi + \int_x^L \frac{1}{(\xi-x)^\alpha} \frac{d^2 u(\xi)}{d\xi^2} d\xi \right\} = 2 \frac{d^2 u(x)}{dx^2} \tag{45}$$

which proves that the curvature at x can be obtained from the integral of the weighted curvatures at positions ξ .

Again, when α differs from one, the integral involves larger characteristic integration domains and the final integral does not reduce to a local expression.

If we come back to expression (42), and apply the derivative using Leibniz's rule

$$\frac{d}{dx} Q_*^\alpha(x) = \frac{1}{2}K \frac{\alpha}{\Gamma(1-\alpha)} \left\{ \int_0^x \frac{1}{(x-\xi)^{\alpha+1}} \frac{du(\xi)}{d\xi} d\xi - \int_x^L \frac{1}{(\xi-x)^{\alpha+1}} \frac{du(\xi)}{d\xi} d\xi \right\} \tag{46}$$

As before, if we consider both integrals in the limit case $\alpha \approx 1$ and assume that the main contribution to both integrals occurs in the interval $[x-\epsilon/2, x+\epsilon/2]$, it follows

$$\begin{aligned} & \int_0^x \frac{1}{(x-\xi)^2} \frac{du(\xi)}{d\xi} d\xi - \int_x^L \frac{1}{(\xi-x)^2} \frac{du(\xi)}{d\xi} d\xi \\ & \approx \int_{x-\epsilon/2}^x \frac{1}{(x-\xi)^2} \frac{du(\xi)}{d\xi} d\xi - \int_x^{x+\epsilon/2} \frac{1}{(\xi-x)^2} \frac{du(\xi)}{d\xi} d\xi \approx \frac{2}{\epsilon} \left(\left. \frac{du(\xi)}{d\xi} \right|_{x-\frac{\epsilon}{2}} - \left. \frac{du(\xi)}{d\xi} \right|_{x+\frac{\epsilon}{2}} \right) \end{aligned} \tag{47}$$

Now, by expressing both derivatives from the ones existing at $x-\epsilon$, x and $x+\epsilon$, it results

$$\frac{2}{\epsilon} \left(\left. \frac{du(\xi)}{d\xi} \right|_{x-\frac{\epsilon}{2}} - \left. \frac{du(\xi)}{d\xi} \right|_{x+\frac{\epsilon}{2}} \right) = \frac{1}{\epsilon} \left(\left. \frac{du(\xi)}{d\xi} \right|_{x-\epsilon} - \left. \frac{du(\xi)}{d\xi} \right|_{x+\epsilon} \right) \approx -2 \frac{d^2 u(x)}{dx^2} \tag{48}$$

When α differs from one, the previous discrete approximation is not valid anymore; however, the discrete expression of both integrals in (46) reads

$$\frac{d}{dx} Q_*^\alpha(x) = \frac{1}{2}K \frac{\alpha}{\Gamma(1-\alpha)} \left\{ \sum_i \frac{1}{(x-i\epsilon)^{\alpha+1}} \left. \frac{du(\xi)}{d\xi} \right|_{\xi=x-i\epsilon} \epsilon - \sum_i \frac{1}{(x+i\epsilon)^{\alpha+1}} \left. \frac{du(\xi)}{d\xi} \right|_{\xi=x+i\epsilon} \epsilon \right\} \tag{49}$$

or grouping

$$\frac{d}{dx} Q_*^\alpha(x) = \frac{1}{2}K \frac{\alpha}{\Gamma(1-\alpha)} \sum_i \beta_i \frac{1}{2i\epsilon} \left\{ \left. \frac{du(\xi)}{d\xi} \right|_{\xi=x-i\epsilon} - \left. \frac{du(\xi)}{d\xi} \right|_{\xi=x+i\epsilon} \right\} \approx -\frac{1}{2}K \frac{\alpha}{\Gamma(1-\alpha)} \sum_i \beta_i C_i(x) \tag{50}$$

where

$$C_i(x) = \frac{\left. \frac{du(\xi)}{d\xi} \right|_{\xi=x+i\epsilon} - \left. \frac{du(\xi)}{d\xi} \right|_{\xi=x-i\epsilon}}{2i\epsilon} \quad (51)$$

which results in a sort of multi-scale curvatures C_i all them evaluated at position x and all them contributing to the solution at position x .

5. Discussion and conclusions

After the previous discussion on the physical content of standard and anomalous diffusion, the last considered under two different perspectives, the ones related to the Riemann–Liouville and Caputo fractional derivatives, the integral nature of diffusion based on these descriptions seems established. When the derivative considered in the flux definition is integer, the integral collapses into a local standard gradient (defining standard flux) or a local standard curvature when applying the divergence of the flux imposed by the balance equation. The remaining question concerns the physics that implies the existence of a non-integer derivative.

A natural explanation consists in assuming that it emerges from larger particle flights than the ones concerned by standard diffusion. For example, when considering Levy flights, the jump length variance diverges.

By using the Caputo formulation, which considers the flux at position x from the contribution of a sequence of gradients involving different characteristic lengths (discrete or continuously distributed), one could expect that, in the presence of multi-scale or fractal media, the flux at position x is composed by the contribution of the different-scale fluxes, justifying the integral expression.

In the case when considering almost one-dimensional media, particles at position x exhibit a spectrum of correlated behavior, and consequently again the gradients involved in the fluxes should concern different characteristic lengths, explaining once more the integral expression of the fluxes. When dimensionality increases, long-distance correlations disappear, because of the interactions coming from the new dimension(s) and consequently physics regains its locality.

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