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

On the physical interpretation of fractional diffusion

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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, anormal 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.

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

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

and

$$\rho(x, t+\tau) = \int\limits_{\mathbb{R}} \rho(x+\Delta, t)\phi(\Delta)\,\mathrm{d}\Delta \tag{2}$$

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

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

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

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

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

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

or

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

If we define the diffusion coefficient D as

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

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

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

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 $\Delta x \to 0$ and $\Delta t \to 0$ 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

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