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Fractional calculus in hydrologic modeling: A numerical perspective

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ABSTRACT

Fractional derivatives can be viewed either as handy extensions of classical calculus or, more deeply, as mathematical operators defined by natural phenomena. This follows the view that the diffusion equation is defined as the governing equation of a Brownian motion. In this paper, we emphasize that fractional derivatives come from the governing equations of stable Lévy motion, and that fractional integration is the corresponding inverse operator. Fractional integration, and its multi-dimensional extensions derived in this way, are intimately tied to fractional Brownian (and Lévy) motions and noises. By following these general principles, we discuss the Eulerian and Lagrangian numerical solutions to fractional partial differential equations, and Eulerian methods for stochastic integrals. These numerical approximations illuminate the essential nature of the fractional calculus.

1. Introduction

The term "fractional calculus" refers to the generalization of integer-order derivatives and integrals to rational order. This topic was first broached by L'Hopital and Leibniz after the latter's co-invention of calculus in the 1700s (see the excellent history by Oldham and Spanier [1]). In fact, the operators can be extended to complex as well as real order, so the "fractional" label is a minor historical misnomer.

Fractional calculus was primarily a mathematical curiosity for centuries (see examples in [1,2]). For example, when Heaviside would take the "square root" of both sides of a diffusion equation, he was generating a 1/2-order time derivative. Some of the first physical applications were by geophysicists describing material somewhere between elastic (Hooke's linear relationship between stress and strain) and viscous (described by Newton's stress proportional to strain rate). In his work on this area starting in the 1960s, geophysicist Michele Caputo derived the fractional derivative that carries his name. Benoit Mandelbrot's work on fractional Brownian motion and geophysical time series starting in the 1960s implicitly used fractional-order integration.

In the 1990s, a resurgence of interest surrounded the application of fractional derivatives in the model equations of anomalous diffusion (see [3] for an extensive review). At the same time, an understanding of the importance of general non-locality in upscaled transport in heterogeneous aquifer material emerged [4,5]. The non-locality is defined by operators that account for (integrate) the concentrations at previous times and/or large regions of space. These studies were based on the simple idea that the concentration change at some collection point (a plane or well) depended on contributions from potentially large distances upstream and/or the concentration loading history for some time in the past. Formally, the non-locality arises when the underlying velocity field is uncertain and correlation scales are significantly large compared to the scale of observation [6]. Upscaled descriptions of transport lose detailed velocity information that is transferred to the non-local operators.

One attempt to incorporate spatial non-locality in a tractable form assumed a set of weights that decayed as a power-law [7–9], which forms the definition of a fractional-order dispersion term. This formulation assumed that the concentration change at some point depended on upstream concentrations, and the dependence decayed like a power law of the distance. Temporal non-locality, in which concentration change at a point depends on the prior concentration "loading" is the basis for hydrologic applications of continuous time random walks (CTRW). The CTRW were shown to define temporal fractional derivatives when the weighting of prior concentration decayed like a power-law (see the extensive review by Metzler and Klafter [3]). A few years later, the formal link between two-state (mobile/immobile) multi-rate mass transfer equations [10,11] and temporally fractional-order models was made [12,13]. This accounts for solute loading into relatively impermeable material that slowly releases the solute after the bulk of a plume has passed.

Forays into fractional calculus in multiple dimensions showed that the fractional derivatives could be extended in ways significantly different than classical cases. The derivative operators

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were defined by the underlying diffusion process of Lévy motion, which could have different scaling rates and skewness in different directions. The derivative operators inherit the different orders and descriptions of skewness in all directions. Because of the link between derivatives and integrals, these extensions can be transferred to any system that uses fractional integrals. The most common hydrologic application of fractional integration is the generation of fractional Brownian motion as a representation of aquifer material with long-range correlation structure. Using the inverses of the newly defined fractional derivatives gave new tools to extend the classical fractional Brownian motion to more closely represent anisotropic aquifer structure [14].

Because the fractional derivative and integrals are defined as convolution operators, they are easy to implement using standard numerical techniques. In addition, because the fractional diffusion equations that generate the derivative operators are based on the motion of a single particle, the classical random walk particle tracking (RWPT) techniques are well-suited to solve the fractional advection–dispersion transport equations. We exploit the numerical implementations as a vehicle to define and solve to fractional-order differential and integral equations.

The paper is organized in three main sections dealing with fractional space derivatives (Section 2), fractional time derivatives (Section 3), and fractional integrals (Section 5). Within the two derivative sections, we outline how the diffusion equation, and its fractional-order counterparts, are defined by the stochastic processes that they describe. We show how the equations naturally induce both their Eulerian (Section 2.5) and Lagrangian (Section 2.6) numerical approximations. In Section 4 we briefly summarize how the fractional transport equations have been applied to contaminant transport problems in surface and subsurface hydrology. We then show in Section 5 how the inverse of the fractional derivative operators define the fractional integrals in multiple dimensions, and how these integrals can be used to generate conditioned, multi-scaling, random aquifer facsimiles. We close with conclusions and recommendations for future work in Section 6.

2. Markovian diffusions and fractional space derivatives

There are several forms of fractional derivatives that are distinguished by the domain over which they operate. Because they are non-local operators, they "look" for values from a certain distance ahead or behind for information. For spatial processes it may be correct to look ahead and/or behind (or at any angle) over all space. Temporal information is only used after some starting time, so the domain of interest is positive time only. We use these distinctions to explain the association of the different operators to different behaviors in diffusions based on random walks.

The starting point for all of the generalizations is classical Brownian motion. It is well known that Brownian motion $B(t)$ is the limit Markov (memoryless) process of finite-variance random walks with short-range correlation [15,16]. This makes Brownian motion an attractive model for transport of passive tracers in surface and ground water: the exact nature of the individual motions is not particularly important in the long-term. The central limit theorem dictates that all finite-variance motions converge toward the Gaussian limit distribution. It is precisely this property that has made Brownian motion an attractive and useful model of macrodispersion in aquifers. Even with non-Gaussian particle motions, the long term transport tends toward the Gaussian limit distribution (for perhaps the earliest experimental example see Taylor [17]).

If $B(t)$ denotes the location of a particle in one-dimensional space x at time t then the density of the location $p(x,t)$ is given by

$$p(x,t) = \frac{1}{\sqrt{4\pi D t}} \exp\left(\frac{-x^2}{4Dt}\right), \tag{1}$$

where D is half the variance of each motion size divided by the mean motion time. Throughout this paper, we will use Fourier $f(k) \equiv \int e^{-ikx} f(x)dx$ and Laplace $f(s) \equiv \int e^{-st} f(t)$ transforms, where it is understood for notational simplicity that $f(x) \Leftrightarrow f(k)$ and $f(t) \Leftrightarrow f(s)$ are transform pairs, not the same functions.

To connect the diffusion equation with Brownian motion, note that the Fourier transform (FT) of (1) is $p(k,t) = \exp(tD(ik)^2)$, with time derivative

$$\frac{dp(k,t)}{dt} = D(ik)^2 \exp(tD(ik)^2) = D(ik)^2 p(k,t). \tag{2}$$

A property of Fourier transforms of integer-order derivatives is that $(ik)^n f(k) \Leftrightarrow d^n f(x)/dx^n$, so that the inverse transform of the previous equation becomes

$$\frac{\partial p(x,t)}{\partial t} = D\frac{\partial^2}{\partial x^2} p(k,t). \tag{3}$$

In a more general way that will be useful shortly, we can write the FT of the Brownian motion density as $p(k,t) = \exp(tA(k))$, where the function of the wavenumber $A(k) = D(ik)^2$, then following the same procedure the "inverse FT" of $A(k)$ defines the linear space operator in the Cauchy equations

$$\frac{dp(k,t)}{dt} = A(k)p(k,t) \tag{4}$$

with inverse FT

$$\frac{dp(x,t)}{dt} = \int A(x)p(x-\xi,t)d\xi \equiv A_x p(x,t), \tag{5}$$

where the $A_x()$ denotes the linear space operator defined by convolution with $A(x)$, the inverse FT of $A(k)$. Here we use the fact that the product of two functions $A(k)p(k,t)$ in Fourier space is a convolution in real space. This convolution, in turn, specifies an operation on the function $p(x,t)$ in real space. For example $(ik)^2 \Leftrightarrow d^2/dx^2$ represent the pair $A(k) \Leftrightarrow A_x$ for Brownian motion. This convolution machinery can be used to explain the diffusion equation for Brownian motion, because the function $(ik)^2$ is the (distributional) FT of the second derivative of the Dirac delta function. The Dirac delta function $\delta(x-a)$ for some constant shift a is a "generalized function" (also called a distribution) defined by

$$\int \delta(x-a)f(x)dx = f(a). \tag{6}$$

Its derivatives are defined via integration by parts:

$$\int \delta^{(n)}(\xi)f(x-\xi)d\xi = \int \delta(\xi)f^{(n)}(x-\xi)d\xi. \tag{7}$$

Because the values of $f(x)$ for $x \neq a$ do not affect the integral (6), we might say that

$$\delta(x-a) = \begin{cases} \infty & \text{if } x = a, \\ 0 & \text{otherwise}, \end{cases} \tag{8}$$

where $\int \delta(x)dx = 1$, so that the infinity at $x = a$ is tamed by integration. Another intuitive definition of the Dirac function is that it is the limit of a Gaussian density function with mean a as the variance tends toward zero, i.e., the Dirac delta is like the probability density "function" of the constant number a.

Taking $f(x) = e^{-ikx}$ in Eq. (6) shows that the FT of $\delta(x-0)$ equals 1. Then the FT of $\delta''(x)$ is $(ik)^2 \times 1$, so that multiplying the FT by $(ik)^2$ is equivalent to convolution with $\delta''(x)$. Therefore, Brownian motion, by virtue of the FT of its density function, defines the diffusion equation. This is the sole connection between the diffusion equation and Brownian motion. The notion that a concentration gradient "drives" a diffusion by physical means was dispelled by Einstein [18] and Crank [19] in their seminal work. The extension of the probability distribution for a single particle, $p(x,t)$ to concentration for a large