



Anomalous diffusion modeling by fractal and fractional derivatives[☆]

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ABSTRACT

This paper makes an attempt to develop a fractal derivative model of anomalous diffusion. We also derive the fundamental solution of the fractal derivative equation for anomalous diffusion, which characterizes a clear power law. This new model is compared with the corresponding fractional derivative model in terms of computational efficiency, diffusion velocity, and heavy tail property. The merits and distinctions of these two models of anomalous diffusion are then summarized.

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1. Introduction

In recent years, the phenomena of anomalous diffusion have been observed in many fields, such as those of turbulence, seepage in porous media, pollution control [1–5]. Although the demand for appropriate mathematical models is high from biomechanics to geophysics to acoustics, the differential equation modelling of anomalous diffusion has long been a perplexing mathematical physics issue.

Nonlinear modelling is a popular approach to depicting a variety of complex anomalous diffusion phenomena. However, it is mathematically very difficult to analyze and computationally very expensive to simulate. In addition, the nonlinear models often require some parameters unavailable from experiment or field measurements. As alternative approaches, in recent decades the fractal and fractional derivatives have been found effective in modelling anomalous diffusion processes [2,3]. The advantage of the fractal or the fractional derivative models over the standard integer-order derivative models is in that the former can describe very well the inherent abnormal-exponential or heavy tail decay processes.

From the viewpoint of statistical physics, the normal diffusion underlies the well-known Brownian motion of the particles. The probability density function (PDF) in space, evolving in time, which governs the Brownian motion, is of the Gaussian type whose variance is proportional to the first power of time. In contrast, a number of evolution equations have been proposed in recent decades for describing anomalous diffusion, in which the variance is no longer proportional to the first power of time. One of the most popular statistical models of anomalous diffusion is the continuous time random walk model (CTRW), which corresponds to the fractional diffusion equation underlying the Lévy diffusion process [6,7]. It is worthwhile to note that the parameters of the fractional derivative models have clear physical significance and are easy to get from a data fitting of experimental or field measurements. In addition, the models of this type are also mathematically easy to analyze. However, like nonlinear equation models, these models are not computationally cheap and are also of a phenomenological description which does not necessarily reflect the physical mechanism behind the scenes.

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On the other hand, Chen [8] recently introduced a fractal derivative from the fractal concept and applied it to model a variety of power law scaling phenomena, such as turbulence, fractional quantum mechanics, and anomalous diffusion. It was found that the well-known stretched Gaussian distribution is the analytical solution of the fractal derivative anomalous diffusion equation [9,10].

However, to the best of our knowledge, in-depth analysis and comparisons of the fractal and the fractional derivative models of anomalous diffusion have not been reported in the literature. Through theoretical analysis and numerical experiments, this study makes an attempt to investigate the merits and demerits of these two modelling approaches.

2. Definitions of the fractal derivative and the fractional derivative

In this study, we employ the fractal derivative defined in Ref. [8],

$$\frac{\partial u}{\partial t^\alpha} = \lim_{t_1 \rightarrow t} \frac{u(t_1) - u(t)}{t_1^\alpha - t^\alpha}, \quad 0 < \alpha. \tag{1}$$

A more generalized definition is given by

$$\frac{\partial u^\beta}{\partial t^\alpha} = \lim_{t_1 \rightarrow t} \frac{u^\beta(t_1) - u^\beta(t)}{t_1^\alpha - t^\alpha}, \quad 0 < \alpha, 0 < \beta. \tag{2}$$

There are a few different definitions of fractional derivatives such as Grunwald–Letnikov, Riemann–Liouville, Caputo, Riesz–Feller fractional derivatives [11,12], and the fractional Laplacian [13], all of which have an underlying relationship. In the real-world applications, the Caputo fractional derivative in time is mostly used and is given by

$$\frac{d^p f(t)}{dt^p} = \frac{1}{\Gamma(m - \alpha)} \int_0^t (t - \tau)^{m-1-p} f^{(m)}(\tau) d\tau, \quad (m - 1 \leq p < m), \tag{3}$$

where p is the derivative order, and Γ denotes the Gamma function.

The essential difference of the fractal and the fractional derivatives lies in the former being a local operator, while the latter is a global operator. However, regardless of whether the fractal or the fractional derivative approach is used, the integer-order derivative is simply a limited case.

3. Theoretical analysis

3.1. The fractal derivative model

For simplicity, we restrict our attention to a one-dimensional diffusion process. The fractal derivative model of anomalous diffusion is stated as

$$\begin{cases} \frac{\partial u(x, t)}{\partial t^\alpha} = D \frac{\partial}{\partial x^\beta} \left(\frac{\partial u(x, t)}{\partial x^\beta} \right) t > 0, & -\infty < x < +\infty \\ u(x, 0) = \delta(x), \end{cases} \tag{4}$$

where $0 < \alpha < 2, 0 < \beta \leq 1, D$ is a diffusion coefficient, and $\delta(x)$ represents the delta function.

In order to obtain the fundamental solution of (4), we apply the following variable transforms:

$$\begin{cases} \hat{t} = t^\alpha \\ \hat{x} = x^\beta. \end{cases} \tag{5}$$

(4) is transformed into a normal diffusion equation in the translated variable system. The fundamental solution of (4) is found to be in the form of a stretched Gaussian distribution as shown below [8,14]:

$$u(x, t) = t^{-\alpha/2} G_\beta \left(\frac{x}{t^{\alpha/2\beta}} \right). \tag{6}$$

In this study, the stretched Gaussian kernel is defined as

$$G_\beta(p) = \frac{1}{2\sqrt{\pi D}} e^{-p^{2\beta}/4D}. \tag{7}$$

Expression (6) can be interpreted as a time-dependent spatial probability density function (PDF) which yields the stretched Gaussian distribution evolving in time. By using (6), we can immediately deduce the scaling of the mean square deviation

$$\langle x^2(t) \rangle_{\alpha, \beta} = \int x^2 t^{-\alpha/2} G_\beta \left(\frac{x}{t^{\alpha/2\beta}} \right) dx. \tag{8}$$

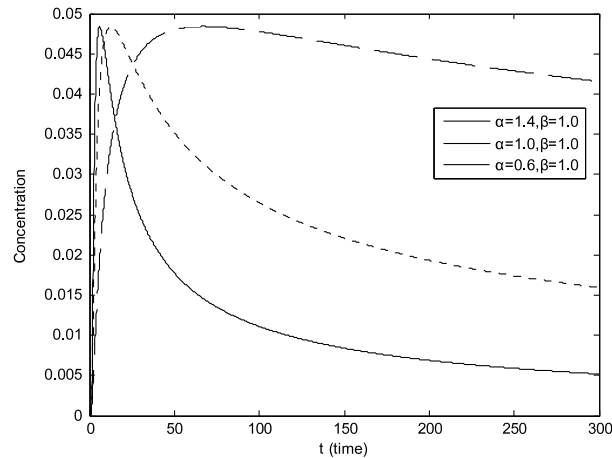


Fig. 1. Anomalous diffusion at $x = 0.5$; thick dashed line: $\alpha = 0.6, \beta = 1.0$, dotted line: $\alpha = 1.0, \beta = 1.0$, thick solid line: $\alpha = 1.4, \beta = 1.0$.

With the substitution $p = x/t^{\alpha/2\beta}$, we get

$$\langle x^2(t) \rangle_{\alpha,\beta} = N_{\alpha,\beta} t^{(3\alpha-\alpha\beta)/2\beta}, \tag{9}$$

where $N_{\alpha,\beta} = \int p^2 G_{\beta}(p) dp$.

It should be noted that when $\alpha = \beta = 1$, (9) is simplified to a normal diffusion process which obeys Fick’s second law $\langle x^2(t) \rangle \propto t$. Otherwise, (9) represents a sub-diffusion process when $\alpha < 2\beta(3 - \beta)$ and a super-diffusion process when $\alpha > 2\beta(3 - \beta)$. Fig. 1 shows the diffusion curves with different parameters α, β .

3.2. The fractional derivative model

The fractional derivative model of anomalous diffusion is given by

$$\begin{cases} \frac{\partial^\gamma u(x, t)}{\partial t^\gamma} = d \frac{\partial^\eta u(x, t)}{\partial |x|^\eta} t > 0, & -\infty < x < +\infty, 0 < \gamma, \eta \leq 2 \\ u(x, 0) = \delta(x). \end{cases} \tag{10}$$

If $\gamma = 1, \eta = 2$, then it becomes a normal diffusion equation. In the Fourier–Laplace domain, (10) can be translated into the following form:

$$s^\gamma \hat{u}(k, s) - s^{\gamma-1} = -d |k|^\eta \hat{u}(k, s), \quad 0 < \gamma \leq 1, 0 < \eta \leq 2, \tag{11}$$

The above expression corresponds to the Riesz fractional derivative in space $\partial^\eta / \partial |x|^\eta = D_{|x|}^\eta \rightarrow -|k|^\eta$ and the Caputo fractional derivative in time $d^\gamma u(x, t) / dt^\gamma \rightarrow s^\gamma \bar{u}(x, s) - s^{\gamma-1}$.

The solution of (11) in the Fourier–Laplace domain is stated as

$$\hat{u}(k, s) = s^{\gamma-1} / (s^\gamma + d |k|^\eta), \quad s > 0, k \in R. \tag{12}$$

According to Refs. [15–17], if $d = 1$, the fundamental solution of (10) can be expressed as

$$u(x, t) = t^{-\gamma/\eta} K_{\gamma,\eta}^\theta \left(\frac{x}{t^{\gamma/\eta}} \right), \quad 0 < \gamma \leq 2, 0 < \eta \leq 2, \tag{13}$$

where the K function is stated as

$$K_{\gamma,\eta}^\theta(x) = \frac{1}{\gamma x} \frac{1}{2\pi i} \int_{\mu-i\infty}^{\mu+i\infty} \frac{\Gamma(s/\gamma) \Gamma(1-s/\gamma) \Gamma(1-s)}{\Gamma(1-\eta s/\gamma) \Gamma(\rho s) \Gamma(1-\rho s)} x^s ds, \tag{14}$$

where μ, ρ are coefficients.

Substituting $p = x/t^{\gamma/\eta}$ into (13) yields

$$\langle x^2(t) \rangle_{\gamma,\eta} = M_{\gamma,\eta} t^{2\gamma/\eta}, \tag{15}$$

where $M_{\gamma,\eta} = \int p^2 K_{\gamma,\eta}(p) dp$.

Eq. (15), which includes the fractional derivative orders γ and η , indicates a sub-diffusion when $2\gamma < \eta$, a normal diffusion when $2\gamma = \eta$, and a super-diffusion when $2\gamma > \eta$.

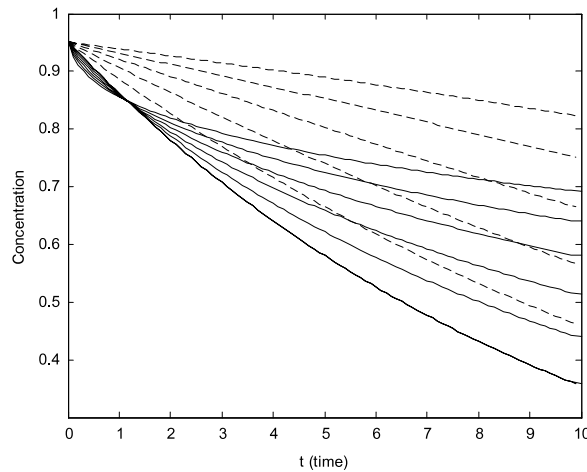


Fig. 2. Diffusion image at $x = 0.6$; dotted line: time fractal model with different orders, from top to bottom: $\alpha = 0.5, 0.6, 0.7, 0.8, 0.9, 1.0$; solid line: time fractional model with different orders, from top to bottom: $\gamma = 0.5, 0.6, 0.7, 0.8, 0.9, 1.0$.

We should mention that if $\gamma = 1, 0 < \eta < 2$, then (10) becomes a spatial fractional derivative equation. Its Fourier transform is given by

$$\hat{u} = \exp(d(ik)^\eta t). \tag{16}$$

The expression (16) can be interpreted as an α -stable probability density function characterizing a power law tail. A generalized non-local Fick’s law can be derived from the spatial fractional diffusion equation underlying the Lévy–Feller statistics [18–22].

4. Numerical experiments

In this section, we focus on the time fractal and the time fractional diffusion equations having derivative order no bigger than 1, which are known to describe sub-diffusive processes. The time fractal derivative model is given by

$$\begin{cases} \frac{\partial u(x, t)}{\partial t^\alpha} = \frac{\partial^2 u(x, t)}{\partial x^2}, & 0 < x < L, t > 0, 0 < \alpha \leq 1 \\ u(0, t) = u(L, t) = 0 \\ u(x, t) = \sin \frac{x\pi}{L}. \end{cases} \tag{17}$$

The time fractional diffusion equation is stated as

$$\begin{cases} \frac{d^\gamma u(x, t)}{dt^\gamma} = \frac{\partial^2 u(x, t)}{\partial x^2}, & 0 < x < L, t > 0, 0 < \gamma \leq 1 \\ u(0, t) = u(L, t) = 0 \\ u(x, 0) = \sin \frac{x\pi}{L}. \end{cases} \tag{18}$$

In the (18), $d^\gamma u(x, t)/dt^\gamma$ represents the fractional derivative of the Caputo definition.

In this study, we use the Crank–Nicholson finite difference discretization scheme for the above two models. It is known that this numerical scheme is unconditionally stable, convergent [7,23], and has numerical accuracy of $(2 - \gamma)$ order for the fractional derivative equation [24]. We can also validate that it is unconditionally stable and convergent for the fractal derivative equation.

From Figs. 2 and 3, we have found that the diffusion velocity in the time fractional derivative model is much higher than that of the time fractal derivative model in the interval $t \in (0, 10]$. In the time fractal model, the bigger the fractal derivative order α , the faster the diffusion velocity. In contrast, in the time fractional model, the bigger the order γ , the slower the diffusion rate change in the initial interval $t \in (0, 1]$. But in $t \in [2, 10]$, the diffusion rate increases with the growth of γ . On the other hand, though both models display different diffusion rates which are slower than that of normal diffusion and asymptotic to a power function in the long term, the time fractional derivative model exhibits a more prominent heavy tail than the time fractal derivative model. In addition, if we employ the space fractal derivative model, it will exhibit the remarkable skewness property in the spatial domain.

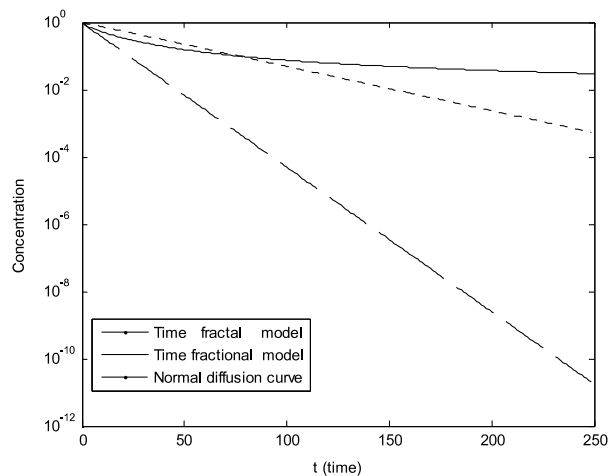


Fig. 3. Diffusion image at $x = 0.6$ in logarithmic coordinates; $\alpha = 0.8$ in the time fractal model (dotted line); $\gamma = 0.8$ in the time fractional model (solid line).

5. Conclusions

From a statistical viewpoint, the fractal diffusion equation underlies the stretched Gaussian process, while the fractional diffusion equation reflects the Lévy process. Although both models can characterize the power law phenomena of anomalous diffusion, this study has observed some notable differences in diffusion rate and heavy tail behaviours, etc. Since the fractal derivative is a local operator, unlike the global fractional derivative operator, the numerical solution of fractal derivative equations can be carried out by standard numerical techniques for the integer-order derivative equations and thus is far more mathematically simple and computationally efficient than that of fractional derivative equations.

It should be noted that both models can depict a variety of kinds of anomalous diffusion processes, but the particular application areas of the two modelling approaches are still unclear. There are also some unresolved issues in this study such as the complete mathematical foundation of the fractal derivative, the physical mechanism of the descriptive models, to mention but a few. Therefore, further study of these open problems is still under way.

References

- [1] W. Chen, A speculative study of 2/3-order fractional Laplacian modeling of turbulence: Some thoughts and conjectures, *Chaos* 16 (2006) 023126.
- [2] M.M. Meerschaert, C. Tadjeran, Finite difference approximations for fractional advection–dispersion flow equations, *Journal of Computational and Applied Mathematics* 172 (2004) 65–77.
- [3] A.A. Greenenko, A.V. Chechkin, N.F. Shul'ga, Anomalous diffusion and Lévy flights in channelling, *Physics Letters A* 324 (2004) 82–85.
- [4] B.M. Schulz, M. Schulz, Numerical investigations of anomalous diffusion effects in glasses, *Journal of Non-Crystalline Solids* 352 (2006) 4884–4887.
- [5] V.V. Anh, J.M. Angulo, M.D. Ruiz-Medina, Diffusion on multifractals, *Nonlinear Analysis* 63 (2005) e2043–e2056.
- [6] P. Paradisia, R. Cesari, F. Mainardi, F. Tampieri, The fractional Fick's law for non-local transport processes, *Physica A* 293 (2001) 130–142.
- [7] H. Zhang, F. Liu, V. Anh, Numerical approximation of Lévy–Feller diffusion equation and its probability interpretation, *Journal of Computational and Applied Mathematics* 206 (2007) 1098–1115.
- [8] W. Chen, Time–space fabric underlying anomalous diffusion, *Chaos, Solitons and Fractals* 28 (2006) 923–929.
- [9] W. Chen, Fractional and fractal derivatives modeling of turbulence [J], Arxiv preprint nlin/0511066, 2005.
- [10] R. Kanno, Representation of random walk in fractal space-time, *Physica A* 248 (1998) 165–175.
- [11] I. Podlubny, *Fractional Differential Equation [M]*, Academic press, San Diego, 1999, pp. 50–78.
- [12] R. Gorenflo, F. Mainardi, Random walk models for space-fractional diffusion processes, *Fractional Calculus Applied Analysis* 1 (1998) 167–191.
- [13] W. Chen, S. Holm, Fractional Laplacian time–space models for linear and nonlinear lossy media exhibiting arbitrary frequency power-law dependency, *Journal of the Acoustical Society of America* 115 (4) (2004) 1424–1430.
- [14] M.O. Vlad, R. Metzler, T.F. Nonnenmacher, M.C. Mackey, Universality Classes for asymptotic behavior of relaxation processes in systems with dynamical disorder: Dynamical generalizations of stretched exponential, *J. Math. Phys.* 37 (1996) 2279–2306.
- [15] R. Balescu, V-Langevin equations, continuous time random walks and fractional diffusion, *Chaos, Solitons and Fractals* 34 (2007) 62–80.
- [16] F. Mainardi, Y. Luchko, G. Pagnini, The fundamental solution of the space-time fractional diffusion equation, *Fractional Calculus and Applied Analysis* 4 (2) (2001) 153–192.
- [17] F. Mainardi, G. Pagnini, The role of the Fox–Wright functions in fractional sub-diffusion of distributed order, *Journal of Computational and Applied Mathematics* 207 (2007) 245–257.
- [18] M.M. Meerschaert, C. Tadjeran, Finite difference approximations for two-sided space-fractional partial differential equations, *Applied Numerical Mathematics* 56 (2006) 80–90.
- [19] E.A. Abdel-Rehim, R. Gorenflo, Simulation of the continuous time random walk of the space-fractional diffusion equations, *Journal of Computational and Applied Mathematics* 222 (2) (2008) 274–283.
- [20] R. Gorenflo, A. Vivoli, F. Mainardi, Discrete and continuous random walk models for space-time fractional diffusion, *Nonlinear dynamics* 38 (2004) 101–116.
- [21] S. Abe, S. Thurner, Anomalous diffusion in view of Einstein's 1905 theory of Brownian motion, *Physica A* 356 (2005) 403–407.
- [22] J.-Y. Go, Su-Il Pyun, A review of anomalous diffusion phenomena at fractal interface for diffusion-controlled and non-diffusion-controlled transfer processes, *Journal of Solid State Electrochemistry* 11 (2007) 323–334.
- [23] F. Liu, P. Zhuang, V. Anh, I. Turner, K. Burrage, Stability and convergence of the difference methods for the space–time fractional advection–diffusion equation, *Applied Mathematics and Computation* 191 (2007) 12–20.
- [24] Y. Lin, C. Xu, Finite difference/spectral approximations for the time-fractional diffusion equation, *Journal of Computational Physics* 225 (2007) 1533–1552.