Journal of Computational Physics 293 (2015) 297–311

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Diffusion in heterogeneous media: An iterative scheme for finding approximate solutions to fractional differential equations with time-dependent coefficients

Mauro Bologna [a], Adam Svenkeson [b,c,*], Bruce J. West [d], Paolo Grigolini [b]

[a] Instituto de Alta Investigación, Universidad de Tarapacá, Casilla 6-D, Arica, Chile
[b] Center for Nonlinear Science, University of North Texas, P.O. Box 311427, Denton, TX 76203-1427, USA
[c] Army Research Laboratory, 2800 Powder Mill Road, Adelphi, MD 20783, USA
[d] Information Science Directorate, Army Research Office, Research Triangle Park, NC 27709, USA

A R T I C L E I N F O

Article history:
Received 29 April 2014
Received in revised form 7 August 2014
Accepted 17 August 2014
Available online 23 August 2014

Keywords:
Fractional calculus
Strange kinetics
Anomalous diffusion
Fractional index expansion
Time-dependent coefficients

A B S T R A C T

Diffusion processes in heterogeneous media, and biological systems in particular, are riddled with the difficult theoretical issue of whether the true origin of anomalous behavior is renewal or memory, or a special combination of the two. Accounting for the possible mixture of renewal and memory sources of subdiffusion is challenging from a computational point of view as well. This problem is exacerbated by the limited number of techniques available for solving fractional diffusion equations with time-dependent coefficients. We propose an iterative scheme for solving fractional differential equations with time-dependent coefficients that is based on a parametric expansion in the fractional index. We demonstrate how this method can be used to predict the long-time behavior of nonautonomous fractional differential equations by studying the anomalous diffusion process arising from a mixture of renewal and memory sources.

1. Introduction

Anomalous diffusion has been explained using strange kinetics [1,2]; a term adopted from nonlinear dynamics to emphasize the lack of a characteristic scale in space, time or both in the phenomena of interest. This concept has been used to describe complex physical [3], social [4] and biological [5,6] processes. In the presence of strange kinetics the traditional diffusion equation is replaced with a fractional diffusion equation in order to adequately describe subdiffusion and superdiffusion. An assumption that was made until fairly recently, with little or no discussion in the construction of the equation of motion for classical diffusion was the homogeneity of the ambient fluid in which the diffusing particle (tracer) is embedded. In the case considered herein inhomogeneity results in the diffusion coefficient being time dependent, resulting in a scaled Brownian motion process [7–9]. However before we focus on this technical problem of solving a nonautonomous fractional differential equation in time we provide a general context for fractional diffusion equations.

Höfling and Franosch [6] point out that in cell biology the diffusion of macromolecules and organelles is anomalous with effects such as time-dependent diffusion coefficients, persistent correlations in time, and non-Gaussian spatial displacements occurring as manifestations of macromolecular crowding in cells and in cellular membranes. Leptos et al. [10] conducted

* Corresponding author.
E-mail addresses: mauroh69@gmail.com (M. Bologna), adam.j.svenkeson.ctr@mail.mil (A. Svenkeson), bruce.j.west.civ@mail.mil (B.J. West), grigo@unt.edu (P. Grigolini).

http://dx.doi.org/10.1016/j.jcp.2014.08.027

experiments on the motion of tracers suspended in a fluid of swimming Eukaryotic microorganisms of varying concentrations. The interplay between the inanimate tracer particles and the advection by flows from the swimming microorganisms resulted in their displacement having a self-similar probability density function (*pdf*) with a Gaussian core and exponential tails. A reanalysis of their data by Eckhardt and Zammert [11] shows an excellent fit to a Mittag-Leffler *pdf* derived using the CTRW model of Montroll and Weiss [12]. Zaid et al. [13] present a theoretical study of a simplified tracer–swimmer interaction showing that the non-Gaussian effect of the tails of the *pdf* can be modeled using a fractional diffusion equation.

However most complex biological phenomena do not have fractional diffusion equations that give rise to analytic solutions and therefore they must be solved numerically. There is the rub, most fractional diffusion equations cannot be numerically integrated in a straightforward manner. There is a great deal of subtlety in their integration depending on the fractional indices in space and time and therefore herein we adopt an approach that relies on a new method for obtaining an analytic approximation to the solution of a nonautonomous fractional differential equation.

The equivalence between fractional diffusion in time and subordination [14] makes it possible to bypass the need of designing an efficient numerical algorithm to solve a problem described by fractional derivatives in time [15], insofar as it leads to a procedure resting on ordinary derivative numerical algorithms, supplemented by the assumption that dynamics are frozen for extended time intervals.

However, there are interesting cases where this procedure cannot be applied. Bologna et al. [16] recently studied a diffusion process generated by the joint action of correlated fluctuations and trapping process that by itself would lead to subdiffusion whereas the correlated fluctuations may generate either subdiffusion or superdiffusion. The trapping process, as in Refs. [14] and [15], is simulated by fractional derivatives in time. In this case the subordination procedure is invalidated [16] and recourse to an efficient method of solving the fractional differential equation is required. The present paper is the sequel to that analysis and herein, using iterative techniques, we address the question of how to construct the approximate solution to the fractional diffusion equation describing the joint action of trapping and correlated fluctuations. The results of this study are expected to be of interest to the research work aiming to establish whether the source of anomalous behavior is renewal or memory [5,17].

1.1. Fractional kinetic equations

The general expression for renewal anomalous diffusion is given by the fractional diffusion equation, see for example [3,4,18,19],

$$\frac{\partial^\alpha}{\partial t^\alpha} p(x,t) = D \frac{\partial^\beta}{\partial x^\beta} p(x,t), \qquad p(x,t=0) = \delta(x), \tag{1}$$

with $\alpha \le 1$ and $\beta \le 2$. The condition $\alpha = 1$ and $\beta = 2$ corresponds to the ordinary diffusion equation, which only applies to homogeneous media. Real diffusion processes in complex media are called anomalous since they do not scale in the traditional way and they obey the more general fractional diffusion equation, with $\alpha \ne 1$ and $\beta \ne 2$. The renewal nature of this picture is easily explained metaphorically for both $\alpha < 1$ and $\beta < 2$ using Aesop's fable of the race between the tortoise and the hare [20]. The random walker is the hare who takes long naps intermittently disrupted by very long jumps. In fact, the condition $\alpha < 1$ corresponds to the hare resting at the site with coordinate x for an extended time drawn from a waiting-time *pdf* $\psi(\tau)$ with the time asymptotic inverse power-law structure

$$\psi(\tau) \propto \frac{1}{\tau^{1+\alpha}}. \tag{2}$$

At the end of the n-th rest time interval of length τ_n a new time interval τ_{n+1} is selected, with no correlation with the lengths of the earlier time intervals. Thus, at the end of a very long time interval with no event, the system is renewed through the choice of a new time interval that does not have any correlation with the system's past. The source of anomaly is not given by the memory of the past but by the fact that for $\mu = 1 + \alpha < 2$ the mean waiting time

$$\langle \tau \rangle = \int_0^\infty t \psi(t) dt \tag{3}$$

is infinite. Consequently, longer and longer time intervals are expected to appear between events so as to make $\langle \tau \rangle = \infty$ possible. To avoid ambiguity in our definition of memory we note that while it is true that an individual walker has no memory of the past when making the next step, an increasing fraction of the walkers in an ensemble appears to be immobile as time advances because of the infinite mean waiting time between jumps [21]. In short, there is memory in the evolution of the *pdf*, as made evident by the fractional derivative in time in Eq. (1), but this definition of memory is different from the slowly-decaying correlation between steps of the random walk that we are referring to.

We use the Caputo fractional derivative in time defined in terms of the Laplace transform

$$\mathcal{L}\left[\frac{\partial^\alpha}{\partial t^\alpha} p(x,t); s\right] = s^\alpha \widehat{p}(x,s) - s^{\alpha-1} p(x,0) \tag{4}$$