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NONLOCAL-IN-TIME DYNAMICS AND CROSSOVER OF DIFFUSIVE REGIMES

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Abstract. The aim of this paper is to study a simple nonlocal-in-time dynamic system proposed for the effective modeling of complex diffusive regimes in heterogeneous media. We present its solutions and their commonly studied statistics such as the mean square distance. This interesting model employs a nonlocal operator to replace the conventional first-order time-derivative. It introduces a finite memory effect of a constant length encoded through a kernel function. The nonlocal-in-time operator is related to fractional time derivatives that rely on the entire time-history on one hand, while reduces to, on the other hand, the classical time derivative if the length of the memory window diminishes. This allows us to demonstrate the effectiveness of the nonlocal-in-time model in capturing the crossover widely observed in nature between the initial sub-diffusion and the long time normal diffusion.

Key words. Nonlocal model, nonlocal operators, mean square displacement, sub-diffusion, numerical methods.

1. Introduction

Diffusion is one of the prominent transport mechanisms in nature. A conventional normal diffusion typically refers to a diffusion process with the mean squared displacement changing linearly in time. Over the last few decades, anomalous diffusion has attracted a lot of attention due to its associations with many diffusion processes in heterogeneous media [4, 28], though its origins and relevant mathematical models can take significantly different forms [23, 33, 3, 26]. On one hand, new experimental standards have been called for [32] to obtain more fundamental statistics on anomalous diffusion processes. On the other hand, there are needs for in-depth studies of novel models, which might be non-conventional and nonlocal [33, 10].

The goal of this work is to present a simple dynamic equation that provides an effective description of the diffusion process encompassing different diffusive regimes. This is motivated by some recent experimental reports on the crossover between initial transient sub-diffusion and long time normal diffusion in various settings [17, 36]. The main feature of the proposed model is to incorporate memory effect or time correlations with a finite and fixed horizon length, denoted by $\delta > 0$, across the dynamic process. The memory kernel is constant in space and time so that neither spatial inhomogeneities nor time variations get introduced in the diffusivity coefficients. This is different from the approaches taken in other models of anomalous diffusion like the variable-order fractional differential equation [35, 40, 38] or the diffusing diffusivity model [6, 16, 18]. Very recently, [2] presented an interesting study on the use of different types of fractional differential equations to capture crossovers from the initial superdiffusive regime to later normal and subdiffusive regime. Our findings presented here complement those given in [2] as we are aiming to study the opposite process of changing from subdiffusive to normal regimes. On one hand, our nonlocal in time model is quite elegant: it does

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not require the introduction of a time dependent memory kernel, and it does not involve spatial heterogeneities. On the other hand, the model under consideration here is also very intuitive: due to the fixed memory span, the memory effect plays an dominant role in the whole or a large part of the time history so that the non-Markovian effect is evident during the early time period. As time goes on, however, the fixed memory span becomes less and less significant in comparison with the longer and longer life history. Hence, the process becomes more and more Markovian like. As a result, the transition from sub-diffusion to normal diffusion occurs naturally. A rigorous demonstration of this intuitive picture will be given later in more details. We note that while the nonlocal-in-time diffusion equation may be related to fractional diffusion equations [29, 30, 33] by taking special memory kernels [1], they in general provide a new class of models that effectively serve as a bridge between anomalous diffusion and normal diffusion, with the latter being a limiting case as the horizon length $\delta \to 0$.

Specifically, let Δ be the Laplacian (diffusion) operator in the spatial variable x and $g = g(x,t)$ represent the initial (historical) data, we consider the following nonlocal-in-time diffusion equation for $u = u(x,t)$:

$$\begin{aligned} \mathcal{G}_\delta u &= \Delta u \qquad \forall\, t > 0, \\ u &= g \qquad\ \ \forall\, t \in (-\delta, 0). \end{aligned} \tag{1}$$

The nonlocal operator $\mathcal{G}_\delta$ in (1) is defined by

$$\mathcal{G}_\delta v(t) = \int_0^\delta \frac{v(t) - v(t-s)}{s} \rho_\delta(s)\, ds, \tag{2}$$

where the memory kernel function $\rho_\delta = \rho_\delta(s)$ is assumed to be nonnegative with a compact support in $(0,\delta)$ and is integrable in $(0,\delta)$. In case that $s^{-1}\rho_\delta(s)$ is unbounded only at the origin, the integral in (2) should be interpreted as the limit of the integral of the same integrand over (ϵ,δ) for $\epsilon > 0$ as $\epsilon \to 0$, where such a limit exists in an appropriate mathematical sense.

The nonlocal operator $\mathcal{G}_\delta$ has been discussed in [13, 11, 12], and it forms part of the nonlocal vector calculus [9, 27]. The positive nonlocal horizon parameter δ appearing in (2) represents the memory span. For suitably chosen kernels, as $\delta \to 0$, nonlocal and memory effects diminish, so that the zero-horizon limit of the nonlocal operator $\mathcal{G}_\delta u$ corresponds to the standard first order derivative $\frac{d}{dt}u$. In particular, under the normalization condition

$$\int_0^\delta \rho_\delta(s)\, ds = 1, \tag{3}$$

the kernel function $\rho_\delta(s)$ can be seen as a probabilistic density function(PDF) defined for s in $(0,\delta)$, so that the nonlocal operator (2) can be viewed as a "continuum" average of the backward difference operators over the memory span measured by the horizon $\delta > 0$. The local limit, i.e., the standard derivative, is simply the extreme case where $\rho_\delta(s)$ degenerates into a singular point measure at $s = 0$. In fact, one can see from a formal Taylor expansion that

$$\mathcal{G}_\delta v(t) = \frac{dv}{dt}(t) + \sum_{k=2}^{\infty} \frac{v^{(k)}(t)}{k!} \int_0^\delta (-s)^{k-1} \rho_\delta(s)\, ds = \frac{dv}{dt}(t) + O(\delta) \to \frac{dv}{dt}(t).$$

as $\delta \to 0$. Then the nonlocal-in-time model (1) recovers the following classical (local) diffusion model

$$\partial_t u = \Delta u \qquad \forall\, t > 0, \quad \text{with } u(0) = g(0).$$