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Fractional reaction–diffusion

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Abstract

We derive a fractional reaction–diffusion equation from a continuous-time random walk model with temporal memory and sources. The equation provides a general model for reaction–diffusion phenomena with anomalous diffusion such as occurs in spatially inhomogeneous environments. As a first investigation of this equation we consider the special case of single species fractional reaction–diffusion in one dimension and show that the fractional diffusion does not by itself precipitate a Turing instability. © 2000 Elsevier Science B.V. All rights reserved.

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1. Introduction

In recent years there has been a great deal of interest in fractional diffusion equations [1–6]. These equations arise quite naturally [7,3] in continuous-time random walks with spatial and temporal memories [8–11]. The nature of the diffusion is characterized by the temporal scaling of the mean-square displacement $\langle r^2(t) \rangle \sim t^\gamma$. For standard diffusion $\gamma = 1$, whereas in anomalous sub-diffusion $\gamma < 1$, and in anomalous super-diffusion $\gamma > 1$. Sub-diffusion typically arises in cases where there are spatial or temporal constraints such as occur in fractured and porous media and fractal lattices [12]. Super-diffusion may occur in chaotic or turbulent processes through enhanced transport of particles [13]. The review paper by Klafter et al. [14] provides numerous references to physical phenomena in which anomalous diffusion occurs.

Both types of anomalous diffusion have been unified in continuous-time random walk (CTRW) models with spatial and temporal memories [7]. We restrict the following analysis to the sub-diffusive case which can be obtained from CTRWs with the spatial and temporal probability density functions decoupled [8] and with temporal memory.

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In the next section we derive a fractional diffusion equation with a source term from a continuous time random walk model with temporal memory and sources. In Section 3 we consider the case where the source term is a reaction term and our equation describes a fractional reaction–diffusion equation. A particular solution of this equation in the case of zero flux boundary conditions is the homogeneous steady-state solution. In Section 4 we investigate the linear stability of the homogeneous steady-state solution in the special case of the single species fractional reaction–diffusion equation in one dimension. We find that if the homogeneous steady-state solution is stable in the absence of standard diffusion then it remains stable in the presence of fractional diffusion, hence the fractional diffusion does not by itself precipitate a Turing instability in this system. We conclude with a short summary discussion in Section 5.

2. Continuous-time random walk model with sources

The fractional diffusion equation was first derived in the context of a continuous-time random walk model by Compte [3] building on previous work by Klafter et al. [7]. In our derivation of the fractional diffusion equation with the inclusion of a source term we closely follow the spirit of these earlier investigators but we also point out important distinctions in our approach.

Our starting point is the evolution equation for the number density of walkers, $n(\mathbf{r}, t)$, at position \mathbf{r} and time t in a continuous-time random walk model with a source term, $G(\mathbf{r}, t)$, allowing for the addition or removal of walkers:

$$n(\mathbf{r}, t) = \Phi(t)n(\mathbf{r}, 0) + \sum_{\mathbf{r}'} \int_0^t \Psi(\mathbf{r} - \mathbf{r}', t - t')n(\mathbf{r}', t') dt' + G(\mathbf{r}, t). \quad (1)$$

The function $\Phi(t)$ is the probability that the walkers remain at their starting location after time t ; the second term on the right-hand side represents the number of walkers that arrive at \mathbf{r} at time t , having stepped from locations \mathbf{r}' and times t' ; the third term is our source term which we take to be of the form

$$G(\mathbf{r}, t) = \int_0^t \Phi(t - t')g(\mathbf{r}, t') dt'. \quad (2)$$

The source term represents the number of walkers injected (or removed) at \mathbf{r} at time $t' < t$ which remain (or do not return) at \mathbf{r} after time $t - t'$.

The function $\Psi(\mathbf{r}, t)$ represents the transition probability distribution for a walker to take a step of length \mathbf{r} in the time interval t to $t + dt$. In the case where the time intervals between steps and the lengths of the steps are independent this function can be decoupled [8], i.e.,

$$\Psi(\mathbf{r}, t) = \psi(t)\lambda(\mathbf{r}), \quad (3)$$

where $\lambda(\mathbf{r})$ is the step length distribution function and $\psi(t)$ is the waiting time distribution function for the random times when the walker steps.

Fractional sub-diffusion, for which $\langle \mathbf{r}^2(t) \rangle \sim t^\gamma$ with $0 < \gamma < 1$, is a generic feature of continuous-time random walk models characterized by waiting time distributions with the asymptotic form [10]

$$\psi(t) \sim \frac{t^{-1-\gamma}}{\Gamma(1-\gamma)A(t)}. \quad (4)$$

The function $A(t)$ is slowly varying in the sense that for fixed $\lambda > 0$ [15],

$$\lim_{y \rightarrow \infty} \frac{A(\lambda y)}{A(y)} \sim \lim_{y \rightarrow \infty} \frac{A(\lambda/y)}{A(1/y)} \sim 1.$$

With the incorporation of such a waiting time distribution, the steps involved in the derivation of the fractional reaction–diffusion equation are: (i) take a spatial Fourier transform and a temporal Laplace transform of the evolution equation; (ii) carry out asymptotic expansions for small values of the Fourier variable and the Laplace variable; (iii) take the inverse Fourier and Laplace transforms and utilize the definition of the Riemann–Liouville fractional derivative. We now consider these steps in detail.

Use of the decoupled form of the transition probability distribution, Eq. (3), in the equation of motion, Eq. (1), permits the application of the Fourier and Laplace convolution theorems to simplify the spatial Fourier transform and temporal Laplace transform of this equation. A further simplification follows from the use of Eq. (2) together with the Laplace convolution theorem. The Fourier–Laplace transform of Eq. (1) thus yields,

$$\hat{n}(\mathbf{q}, u) = \hat{\Phi}(u)\hat{n}(\mathbf{q}, 0) + \hat{\psi}(u)\hat{\lambda}(\mathbf{q})\hat{n}(\mathbf{q}, u) + \hat{\Phi}(u)\hat{g}(\mathbf{q}, u), \quad (5)$$

where \mathbf{q} is the Fourier transform variable, u is the Laplace transform variable, a single hat denotes either a Fourier transform or a Laplace transform, and a double hat denotes a Fourier and Laplace transform. The Laplace transform of the survival probability at the current position written as [7]

$$\Phi(t) = 1 - \int_0^t \psi(t') dt'$$

is given by $\hat{\Phi}(u) = 1/u - \hat{\Psi}(u)/u$, so that Eq. (5) may be written in the form

$$u\hat{n}(\mathbf{q}, u) = (1 - \hat{\psi}(u))\hat{n}(\mathbf{q}, 0) + u\hat{\psi}(u)\hat{\lambda}(\mathbf{q})\hat{n}(\mathbf{q}, u) + (1 - \hat{\psi}(u))\hat{g}(\mathbf{q}, u). \quad (6)$$

It is assumed that the (normalized) step length distribution function is an even function and that $\hat{\lambda}(\mathbf{q})$ can be expanded in a power series for small \mathbf{q} up to and including the second moment, i.e.,

$$\hat{\lambda}(\mathbf{q}) = 1 - \frac{q^2 \sigma^2}{2}, \quad (7)$$

where

$$\sigma^2 = \int r^2 \lambda(\mathbf{r}) d\mathbf{r}.$$

The waiting time intervals corresponding to the waiting time distribution, Eq. (4), have infinite mean and variance (indeed all non-zero integer-order moments are infinite).

A Lévy stable distribution exists which has the same asymptotic behaviour as Eq. (4). This distribution has the Laplace transform [15,10];

$$\hat{\psi}(u) = \exp\left(-\frac{u^\gamma}{A(1/u)}\right) \tag{8}$$

with the expansion for small u given by

$$\hat{\psi}(u) \sim 1 - \frac{u^\gamma}{A(1/u)}. \tag{9}$$

The asymptotic result in Eq. (9) can be derived using Tauberian theorems [15,16].

Substitution of the expansions, Eqs. (7) and (9), into Eq. (6) now yields (to leading order)

$$u\hat{n}(\mathbf{q}, u) = \frac{u^\gamma}{A(1/u)}\hat{n}(\mathbf{q}, 0) + u\left(1 - \frac{q^2\sigma^2}{2} - \frac{u^\gamma}{A(1/u)}\right)\hat{n}(\mathbf{q}, u) + \frac{u^\gamma}{A(1/u)}\hat{g}(\mathbf{q}, u). \tag{10}$$

Rearranging terms and carrying out the inverse Fourier transform of Eq. (10) yields

$$u\hat{n}(\mathbf{r}, u) - n(\mathbf{r}, 0) = Cu^{1-\gamma}\nabla^2\hat{n}(\mathbf{r}, u) + \hat{g}(\mathbf{r}, u), \tag{11}$$

where we have defined $C = \sigma^2/2$, and for simplicity, $A(1/u) = 1$. To invert the Laplace transform in this equation, we make use of the result [17]

$$\mathcal{L}\left(\frac{d^\alpha y(t)}{dt^\alpha}\right) = u^\alpha \hat{y}(u) - \left(\frac{d^{\alpha-1}y(t)}{dt^{\alpha-1}}\right)\Big|_{t=0}, \tag{12}$$

where

$$\frac{d^\alpha y(t)}{dt^\alpha} = \frac{d}{dt}\left(\frac{d^{\alpha-1}y(t)}{dt^{\alpha-1}}\right) \tag{13}$$

is the Riemann–Liouville fractional derivative;

$$\frac{d^{\alpha-1}y(t)}{dt^{\alpha-1}} = \frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{y(s)}{(t-s)^\alpha} ds \tag{14}$$

is the Riemann–Liouville fractional integral; and \mathcal{L} denotes the Laplace transform operator. The inverse Laplace transform of Eq. (11) now yields

$$\frac{\partial n(\mathbf{r}, t)}{\partial t} = C\left(\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\nabla^2 n(\mathbf{r}, t) + \mathcal{L}^{-1}\left(\frac{\partial^{-\gamma}}{\partial t^{-\gamma}}\nabla^2 n(\mathbf{r}, t)\Big|_{t=0}\right)\right) + g(\mathbf{r}, t). \tag{15}$$

3. Fractional reaction–diffusion equations

The fractional diffusion equation with a source term, Eq. (15), derived in the previous section in the context of continuous-time random walks, can equally be regarded as a single species fractional reaction–diffusion equation with $g(\mathbf{r}, t) = f(n(\mathbf{r}, t))$ as the reaction term. Explicitly,

$$\frac{\partial n(\mathbf{r}, t)}{\partial t} = C\left(\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}}\nabla^2 n(\mathbf{r}, t) + \mathcal{L}^{-1}\left(\frac{\partial^{-\gamma}}{\partial t^{-\gamma}}\nabla^2 n(\mathbf{r}, t)\Big|_{t=0}\right)\right) + f(n(\mathbf{r}, t)). \tag{16}$$

This fractional reaction–diffusion equation models a reaction–diffusion system in a spatially inhomogeneous environment. The extension to several species fractional reaction–diffusion is immediate by replacing the scalar quantity n by a vector \mathbf{n} , and replacing the scalar reaction term $f(n)$ by a vector field $\mathbf{f}(\mathbf{n})$. The case $\gamma=1$ recovers the standard reaction–diffusion equation.

The first step in finding a general solution for the fractional reaction–diffusion equation, Eq. (16), is to find the solution of the fractional diffusion equation,

$$\frac{\partial n(\mathbf{r}, t)}{\partial t} = C \left(\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} \nabla^2 n(\mathbf{r}, t) + \mathcal{L}^{-1} \left(\frac{\partial^{-\gamma}}{\partial t^{-\gamma}} \nabla^2 n(\mathbf{r}, t) \Big|_{t=0} \right) \right). \quad (17)$$

In this connection, we note that Eq. (17) differs slightly from a previously derived fractional sub-diffusion equation [3] through our inclusion of the term

$$\mathcal{L}^{-1} \left(\frac{\partial^{-\gamma}}{\partial t^{-\gamma}} \nabla^2 n(\mathbf{r}, t) \Big|_{t=0} \right).$$

If this term is not properly included at the outset then attempts to solve the fractional-diffusion equation via the intermediate step of a Laplace transform would be immediately fraught with unphysical terms. In the past such unphysical terms have either been ignored (see for example, Ref. [3]), or circumvented through the introduction of non-standard fractional derivatives such as the Caputo fractional derivative [18].

Closed-form solutions of the fractional sub-diffusion equation involving Fox functions have been obtained on radially symmetric domains $R^n \setminus \{0\}$ under the boundary condition $\lim_{r \rightarrow \infty} n(r, t) \neq \infty$ and the normalization $\langle n(r, t) \rangle = 1$ [19,2]. Our interest is in the zero-flux boundary conditions appropriate to reaction–diffusion systems, i.e., $\nabla n(\mathbf{r}, t) = 0$ on a closed boundary of the reaction–diffusion domain [20].

A particular solution of the fractional reaction–diffusion equation, Eq. (16), which satisfies the zero flux boundary conditions is the homogeneous steady-state solution $n(\mathbf{r}, t) = n^*$ defined by

$$f(n^*) = 0. \quad (18)$$

In the next section we explore the linear stability of this solution in the single species fractional reaction–diffusion equation in one spatial dimension.

4. Single species linear stability analysis in one dimension

One of the most important applications of reaction–diffusion equations has been to describe the formation of spatial patterns [20]. Spatial patterns may arise from Turing instabilities which occur if the homogeneous steady state is linearly stable to small perturbations in the absence of diffusion, but linearly unstable to small perturbations in the presence of diffusion. Turing instabilities cannot occur in the standard single species reaction–diffusion equation in one spatial dimension [20];

$$\frac{\partial n(x, t)}{\partial t} = C \nabla^2 n(x, t) + f(n(x, t)) \quad (19)$$

with zero flux boundary conditions

$$\left. \frac{\partial \Delta n(x, t)}{\partial x} \right|_{\pm L} = 0. \tag{20}$$

It is a simple exercise to show that in the absence of diffusion the time evolution of a small perturbation $\Delta n(x, t)$ about the homogeneous steady state is given by

$$\Delta n(x, t) = \Delta n(x, 0) \exp(f'(n^*)t),$$

whereas in the presence of diffusion the perturbation evolves as

$$\Delta n(x, t) = \sum_{l=0} a_l \cos\left(\frac{l\pi x}{L}\right) \exp\left(-\frac{l^2 \pi^2 C}{L^2} t\right) \exp(f'(n^*)t). \tag{21}$$

The homogeneous steady-state solution is thus linearly stable in either system provided that $f'(n^*) < 0$.

We now consider the possibility of a Turing instability in the single species fractional reaction–diffusion equation in one dimension. Clearly, as above, in the absence of the fractional diffusion, the homogeneous steady-state solution is stable if $f'(n^*) < 0$. The linear equation governing the evolution of a small perturbation in the presence of the fractional diffusion is obtained by substituting $n(x, t) = n^* + \Delta n(x, t)$ into Eq. (16) and retaining linear terms in $\Delta n(x, t)$;

$$\begin{aligned} \frac{\partial \Delta n(x, t)}{\partial t} = & C \left(\frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} \nabla^2 \Delta n(x, t) + \mathcal{L}^{-1} \left(\frac{\partial^{-\gamma}}{\partial t^{-\gamma}} \nabla^2 \Delta n(x, t) \Big|_{t=0} \right) \right) \\ & + f'(n^*) \Delta n(x, t). \end{aligned} \tag{22}$$

We now consider the solution of this equation with zero flux boundary conditions, Eq. (20), and initial perturbation

$$\Delta n(x, 0) = \sum_{l=0} a_l \cos\left(\frac{l\pi x}{L}\right).$$

Applying the Laplace transform, Eq. (12), into Eq. (22), and rearranging terms leads to

$$\frac{\partial^2 \hat{\Delta n}(x, u)}{\partial x^2} - \kappa^2(u) \hat{\Delta n}(x, u) = -u^{\gamma-1} \Delta n(x, 0)/C, \tag{23}$$

where

$$\kappa^2(u) = u^\gamma (1 - u^{-1} f'(n^*)) / C. \tag{24}$$

In the case where the homogeneous steady-state solution is stable in the absence of the fractional diffusion, $f'(n^*) = -|f'(n^*)|$, and hence $\kappa^2(u) \geq 0$. In this case the solution of Eq. (23) is of the form

$$\hat{\Delta n}(x, u) = A(u) e^{\kappa(u)x} + B(u) e^{-\kappa(u)x} + \sum_{l=0} \frac{a_l u^{\gamma-1}}{C(l^2 \pi^2 / L^2 + \kappa^2(u))} \cos\left(\frac{l\pi x}{L}\right). \tag{25}$$

When we apply the zero flux boundary conditions, Eq. (20), this simplifies to

$$\hat{\Delta}n(x, u) = \sum_{l=0}^{\infty} \frac{a_l}{(u + (Cl^2\pi^2/L^2)u^{1-\gamma} + |f'(n^*)|)} \cos\left(\frac{l\pi x}{L}\right). \tag{26}$$

The final step of the stability analysis requires inverting the Laplace transform of Eq. (26). First, we note that with $\gamma = 1$, corresponding to standard reaction–diffusion, the inverse Laplace transform recovers Eq. (21). The inverse Laplace transform in the case $\gamma = 0$ is also straightforward, resulting in another stable solution,

$$\Delta n(x, t) = \sum_{l=0}^{\infty} \alpha_l a_l \cos\left(\frac{l\pi x}{L}\right) \exp(-\alpha_l |f'(n^*)|t), \tag{27}$$

where

$$\alpha_l = \frac{1}{Cl^2\pi^2/L^2 + 1} > 0.$$

The inverse Laplace transform for general γ in the range $0 \leq \gamma \leq 1$ can be obtained in closed form by exploiting properties of the two-parameter Mittag–Leffler function [21]. The general result is

$$\Delta n(x, t) = \sum_{l=0}^{\infty} a_l \cos\left(\frac{l\pi x}{L}\right) \sum_{j=0}^{\infty} \sum_{k=0}^{\infty} \frac{(-|f'(n^*)|t)^k (-Cl^2\pi^2/L^2 t^\gamma)^j (j+k)!}{k! j! \Gamma(k+1+\gamma j)}. \tag{28}$$

To determine the asymptotic behaviour of this expression for large t we first note that

$$\Delta n(x, t) \leq \sum_{l=0}^{\infty} a_l \cos\left(\frac{l\pi x}{L}\right) \sum_{j=0}^{\infty} \sum_{k=0}^{\infty} \frac{(-|f'(n^*)|t)^k (-Cl^2\pi^2/L^2 t^\gamma)^j (j+k)!}{k! j! \Gamma(k+1)}, \tag{29}$$

where the equality holds when $\gamma = 0$. The double sum over k and j in Eq. (29) can be written as a single sum

$$\sum_{k=0}^{\infty} \left(\frac{-|f'(n^*)|^k t^k}{k!} \right) \frac{1}{(Cl^2\pi^2/L^2 + 1)^{k+1}}, \tag{30}$$

by applying the binomial theorem. Hence,

$$\Delta n(x, t) \leq \sum_{l=0}^{\infty} a_l \cos\left(\frac{l\pi x}{L}\right) \left(\frac{1}{(Cl^2\pi^2/L^2)t^\gamma + 1} \right) \exp\left(\frac{-|f'(n^*)|t}{(Cl^2\pi^2/L^2)t^\gamma + 1} \right) \tag{31}$$

and the homogeneous steady-state solution with $f'(n^*) < 0$ is stable for all $0 \leq \gamma \leq 1$. From Eq. (31) it follows that the upper bound on the perturbation solution in the limit $t \rightarrow \infty$ decreases with decreasing γ . Thus, the effect of the fractional diffusion γ is to further stabilize the homogeneous steady-state solution.

5. Discussion

In this paper we derived a fractional diffusion equation with a source term from a continuous-time random walk model in which the walks were characterized by a waiting time distribution with infinite moments. Important new elements of our fractional sub-diffusion equation are; (i) the incorporation of a source term allowing for the possibility of modelling fractional reaction–diffusion phenomena, (ii) an additional term of the form

$$\mathcal{L}^{-1} \left(\frac{\partial^{-\gamma}}{\partial t^{-\gamma}} \nabla^2 n(\mathbf{r}, t) \Big|_{t=0} \right),$$

which permits solutions via Laplace transforms for a range of physically meaningful boundary conditions, including zero flux boundary conditions.

One useful application of our equation is to fractional reaction–diffusion systems, where the source term $g(\mathbf{r}, t)$ is interpreted as a reaction term $f(n(\mathbf{r}, t))$ and the diffusion occurs in an inhomogeneous medium. As a first investigation of this type of system we considered the possibility of a Turing instability-induced spatial pattern in a single species fractional reaction–diffusion system in one space dimension. We found that the addition of fractional diffusion to a stable steady-state solution of the reaction problem does not by itself precipitate a Turing instability. Indeed, the effect of the fractional diffusion is to further stabilize the homogeneous steady-state solution.

The investigation of Turing instability-induced spatial pattern formation in the multi-species fractional reaction–diffusion equation remains an exciting area for future research.

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