

# A fractional Fokker–Planck control framework for subdiffusion processes

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## SUMMARY

An efficient framework for the optimal control of the probability density function of a subdiffusion process is presented. This framework is based on a fractional Fokker–Planck equation that governs the time evolution of the PDF of the subdiffusion process and on tracking objectives of terminal configuration of the desired PDF. The corresponding optimization problems are formulated as a sequence of open-loop optimality systems in a model predictive control strategy. The resulting optimality system with fractional evolution operators is discretized by a suitable scheme that guarantees positivity of the forward solution. The effectiveness of the proposed computational framework is validated with numerical experiments. Copyright © 2015 John Wiley & Sons, Ltd.

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## 1. INTRODUCTION

Modeling and controlling of stochastic processes are a very active research field because of many real-world applications in technology, science, and finance. This research is sustained by a well-established theory of stochastic processes [1–4], which provides tools for the description and the analysis of temporal sequences of random quantities in many practical cases. In recent years, many different stochastic models have been proposed and investigated, which belong to the class of Lévy processes [1, 5], piecewise deterministic processes [3, 6, 7], and anomalous diffusion processes [8–14]. For this purpose, a powerful investigation tool results from the fact that the time evolution of the probability density functions (PDFs) of these processes is governed by Fokker–Planck (FP) equations, which are partial differential equations whose structure depends on the type of the underlying stochastic process; see, for example, [15–17].

The focus of our work is on the control of anomalous diffusion processes. The list of systems displaying anomalous transport is very extensive. It encompasses charge carrier transport in amorphous semiconductors, nuclear magnetic resonance, diffusion in percolative and porous systems, transport on fractal geometries and dynamics of a bead in a polymeric network, and protein conformational dynamics; see [11, 16] and references therein. It is the aim of this paper to contribute to the solution of this problem with the formulation of a powerful computational framework for the optimal control of PDFs associated with subdiffusion processes that is based on the related fractional Fokker–Planck

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(FFP) equations. Specifically, we extend the FP control strategy proposed in [7, 18–20], for Itô processes and piecewise deterministic processes, to the case of anomalous diffusion processes. We remark that this extension is novel and not straightforward. In fact, it provides original contributions to the less explored field of control of anomalous diffusion processes and to optimal control with fractional partial differential equations. Furthermore, we discuss a new discretization of the FFP optimality system resulting from the FFP optimal control formulation.

We consider a subdiffusion process described by the state variable  $Y(t) \in \mathbb{R}$  driven by the following model [10, 21–23]

$$\begin{cases} Y(t) = X(S(t)), \\ dX(\tau) = b(X(\tau); u) d\tau + \sigma(X(\tau)) dB_\tau, \\ X(\tau_0) = X_0, \end{cases} \quad (1)$$

where the variable  $X(\tau) \in \mathbb{R}$  is subject to deterministic infinitesimal increments driven by the drift function  $b$  and to random increments proportional to a Wiener process  $dB_\tau \in \mathbb{R}$  and real dispersion coefficient  $\sigma > 0$ . The inverse-time  $\alpha$ -stable subordinator  $S(t) \in \mathbb{R}$  is defined as a first-passage time process as follows:

$$S(t) = \inf\{\tau, U(\tau) > t\},$$

where  $U$  represents the  $\alpha$ -stable Lévy subordinator. More precisely,  $U$  starts at zero, has independent and stationary increments, and its distribution is given by the following Laplace transform  $E(e^{-kU(\tau)}) = e^{-\tau k^\alpha}$ ,  $\alpha \in (0, 1)$ , [24]. Moreover, the processes  $B(\tau)$  and  $S(t)$  are assumed to be independent.

In (1), we assume that the drift  $b$  is a smooth function of the control  $u \in \mathbb{R}$  and considers the action of the control to drive the subdiffusion process such that its PDF follows a desired trajectory or attains a required terminal configuration. The control tasks are formulated by introducing an objective functional that depends on the state and control variables. However, for non-deterministic processes, the state evolution  $Y$  is random, so that a direct insertion of a stochastic process into a deterministic objective function results into a random variable. For this reason, to obtain a deterministic objective, we pursue an alternative approach based on reformulating the control problem from stochastic to deterministic. To formulate our framework, we remark that the state of an anomalous diffusion process can be completely characterized by the shape of its PDF, whose time evolution is modeled by an FFP equation [11, 16]. Therefore, the formulation of objectives in terms of the PDF and the use of the FFP equation provide a consistent framework to formulate a robust control strategy of subdiffusion processes.

In our computational framework, we consider a subdiffusion process in a time interval, with given initial PDF and the objective of approximating a desired final PDF target with the actual PDF of the state variable at the final time. For realistic implementation purposes, as in [7, 18–20], we assume that the control  $u$  is a piecewise constant function to be determined by an open-loop optimal control scheme. The objective is given by a cost functional consisting of a terminal-time tracking objective and the control cost. The resulting control problem is formulated as the problem to find a controller that minimizes the cost functional within the time interval under the constraint provided by the FFP equation. Further, we apply this control strategy to a sequence of time sub-intervals to construct a fast model predictive control (MPC) scheme [25] of the subdiffusion process. Notice that MPC schemes are among the most widely used control techniques in process control [26].

In the next section, we define a representative subdiffusion process and introduce our framework with an optimal control problem based on the FFP equation. In particular, we discuss the characterization of the optimal solution as the solution of an optimality system with forward and adjoint FFP equations and an optimality condition equation. We remark that given a set of values of the controls, the solution of the forward FFP equation and of the adjoint FFP equation enters in the optimality condition, which provides the gradient along which the controls can be improved towards the optimal value. In Section 3, we discuss the discretization of the forward FFP equation using the Chang–Cooper (CC) scheme [19, 27, 28]. This scheme has been especially designed to provide a stable and second-order accurate discretization while preserving positivity of the density function solution. Further, we extend the CC scheme to the approximation of the adjoint FFP equation

ensuring that the resulting scheme is the algebraic adjoint of the forward system. For the time discretization, we consider second-order backward time-discretization formula such that a space-time second-order accurate solution is obtained. Section 4 is devoted to illustrate the MPC scheme and a nonlinear conjugate gradient (NCG) optimization method to solve the minimization of the objective under the constraint given by the FFP model. In Section 6, we discuss the application of our methodology to the challenging optimal control of the PDF of a fractional Ornstein–Uhlenbeck (OU) process. The results obtained with this application demonstrate the ability of our framework to solve subdiffusion control problems. A section of conclusions completes this work.

## 2. A FRACTIONAL FOKKER–PLANCK CONTROL FRAMEWORK

Denote with  $f(x, t)$  the PDF to find the process  $Y(t)$  at  $x \in \Omega \subset \mathbb{R}$  at time  $t \in (0, T)$ . Associated with (1) is the FFP equation [11, 16] modeling the evolution of the probability density. The FFP equation is as follows:

$$\partial_t f(x, t) - {}_0D_t^{1-\alpha} \left[ \frac{a}{2} \partial_{xx}^2 - \partial_x b(x; u) \right] f(x, t) = 0, \quad (2)$$

$$f(x, 0) = \rho(x), \quad (3)$$

where  $a = \sigma^2$ . In (2), the operator

$${}_0D_t^{1-\alpha} g(t) = \frac{1}{\Gamma(\alpha)} \partial_t \int_0^t (t-s)^{\alpha-1} g(s) ds$$

is the fractional Riemann–Liouville derivative, we assume  $g \in C^1([0, T])$ . In our discussion, the FFP equation is defined on  $Q = \Omega \times (0, T)$ , and we consider a bounded interval  $\Omega \subset \mathbb{R}$  with homogeneous Dirichlet boundary conditions, that is, zero probability, on  $\Sigma = \partial\Omega \times (0, T)$ . Further, we assume that the drift  $b \in C^1(\Omega \times \mathbb{R})$ , and choose the initial PDF  $\rho \in C_0^1(\bar{\Omega}) \cap C^2(\Omega)$ , be non-negative and normalized,  $\int_{\Omega} \rho(y) dy = 1$ . Because we are interested in localized systems, we choose the initial PDF of compact support in  $\Omega$ , such that for a short time horizon, we can assume that the evolving PDF remains of almost compact support. With this setting, we refer to [29–33] concerning existence, uniqueness, and regularity of solutions to our FFP problem. In addition, see [33, 34] for the derivation of classical solutions for the FFP problem with homogeneous Dirichlet boundary conditions on bounded domains. In particular, we have that the solution of the FFP problem for a given  $u$  is unique and defines a mapping  $u \rightarrow f(u)$  that is twice differentiable. For this reason, we also denote the dependence of the PDF solution on  $u$  by  $f = f(u)$ .

Next, to illustrate our control framework, we consider a control problem formulated in the time window  $(0, T)$ . We assume that the initial value of the process  $X_t$  at time  $t = 0$  is known, in the sense that its probability density  $\rho(x)$  is assigned. We formulate the problem to determine a control  $u \in \mathbb{R}^\ell$  such that starting with initial distribution  $\rho$ , the process evolves towards a desired target probability density  $f_d(x)$  at time  $t = T$ . This objective can be formulated by the following differentiable tracking functional

$$J(f, u) := \frac{1}{2} \|f(\cdot, T) - f_d(\cdot)\|_{L^2(\Omega)}^2 + \frac{\nu}{2} |u|^2, \quad (4)$$

where  $|u|^2 = u_1^2 + \dots + u_\ell^2$ .

Now, we remark that in the case where the parameters  $a$  and  $b$  and the control  $u$  do not depend on time, the problems (2)–(3) can be conveniently written in the following Caputo form [31, 35]:

$$\partial_t^\alpha f(x, t) - \left[ \frac{a}{2} \partial_{xx}^2 - \partial_x b(x; u) \right] f(x, t) = 0, \quad (5)$$

$$f(x, 0) = \rho(x), \tag{6}$$

where the operator

$$\partial_t^\alpha g(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} \partial_s g(s) ds \tag{7}$$

is the Caputo derivative. See [21, 23, 36] for a discussion on the relationship between the formulations (2) and (5).

The main advantage of Caputo fractional derivative over the Riemann Liouville fractional derivative is that when solving differential equations involving the former one, it is not necessary to define the fractional order initial conditions. The initial conditions for Caputo derivatives are formally the same as for the standard (non-fractional) differential equations, which are important in applications; see, for example, [35].

With this preparation, we formulate our optimal control problem to find  $u$  that minimizes the objective  $J$  subject to the constraint given by the FFP equation. We have

$$\min J(f, u) := \frac{1}{2} \|f(\cdot, T) - f_d(\cdot)\|_{L^2(\Omega)}^2 + \frac{\nu}{2} |u|^2, \tag{8}$$

$$\partial_t^\alpha f(x, t) - \left[ \frac{a}{2} \partial_{xx}^2 - \partial_x b(x; u) \right] f(x, t) = 0, \tag{9}$$

$$f(x, 0) = \rho(x). \tag{10}$$

Because of the mapping  $u \rightarrow f(u)$ , we can introduce the so-called reduced cost functional  $\hat{J}$  given by

$$\hat{J}(u) = J(f(u), u). \tag{11}$$

Notice that we can use standard arguments to prove existence of a minimizer of  $\hat{J}(u)$ ; see, for example, [37, 38]. In fact, because for a given  $u$  the FFP forward problem has a unique solution  $f = f(u)$  and our tracking functional is strictly convex and weakly sequentially lower semi-continuous, there exists a minimizing subsequence of control functions  $(u_n)$  that converges to a local minimizer (notice that our control space is finite dimensional). We refer to [39] for a more general discussion and references on bilinear control problems.

Next, we discuss the characterization of a solution to (8), (9), and (10) as the first-order optimality conditions of a constrained optimization problem. For this purpose, we introduce the following Lagrange function

$$L(f, u, p) = J(f, u) + \int_0^T \int_\Omega \left( \partial_t^\alpha f(x, t) - \left[ \frac{a}{2} \partial_{xx}^2 - \partial_x b(x; u) \right] f(x, t) \right) q(x, t) (T-t)^{\alpha-1} dx dt, \tag{12}$$

where  $0 < \alpha < 1$  and  $q$  is the adjoint PDF function variable.

The first-order optimality conditions for the optimal control problem are formally derived by equating to zero the Frechét derivatives of the Lagrange function with respect to the set of variables  $(f, u, q)$ ; see, for example, [37]. Because  $L$  is continuously differentiable, we can conveniently compute its derivative with the Gateaux derivative. In particular, we have

$$(\nabla_f L, \delta f) = \lim_{\varepsilon \rightarrow 0^+} \frac{L(f + \varepsilon \delta f, u, q) - L(f, u, q)}{\varepsilon}, \tag{13}$$

where  $\delta f$  satisfies homogeneous boundary and initial conditions.

In our case, the difficulty is to handle the fractional time-derivative term. Therefore, we focus on the computation of the following:

$$\begin{aligned} & \left( \nabla_f \left( \int_0^T \int_{\Omega} \partial_t^\alpha f(x, t) q(x, t) (T - t)^{\alpha-1} dx dt \right), \delta f \right) \\ &= \lim_{\varepsilon \rightarrow 0^+} \frac{1}{\varepsilon} \left\{ \int_0^T \int_{\Omega} \partial_t^\alpha (f(x, t) + \varepsilon \delta f) q(x, t) (T - t)^{\alpha-1} dx dt \right. \\ & \quad \left. - \int_0^T \int_{\Omega} \partial_t^\alpha f(x, t) q(x, t) (T - t)^{\alpha-1} dx dt \right\} \\ &= \int_0^T \int_{\Omega} \partial_t^\alpha (\delta f) q(x, t) (T - t)^{\alpha-1} dx dt = \int_0^T \int_{\Omega} (\delta f) \hat{\partial}_t^\alpha q(x, t) dx dt. \end{aligned}$$

With this choice, we obtain the following adjoint fractional time operator (see the Appendix for further details)

$$\hat{\partial}_t^\alpha q(x, t) := -\frac{(T - t)^{-\alpha}}{\Gamma(1 - \alpha)} \int_t^T \left( \frac{T - s}{s - t} \right)^\alpha \partial_s q(x, s) ds. \quad (14)$$

In summary, we obtain the following optimality system that represents the first-order necessary optimality condition for our constrained optimization problem. We have

$$\begin{aligned} \partial_t^\alpha f(x, t) - \left[ \frac{a}{2} \partial_{xx}^2 - \partial_x b(x; u) \right] f(x, t) &= 0 \quad \text{in } Q \quad (\text{state equation}), \\ f(x, 0) &= \rho(x) \quad \text{in } \Omega \quad (\text{initial condition}), \\ \hat{\partial}_t^\alpha q(x, t) - \left[ \frac{a}{2} \partial_{xx}^2 + b(x; u) \partial_x \right] q(x, t) &= 0 \quad \text{in } Q \quad (\text{adjoint equation}), \\ q(x, T) &= (f_d(x) - f(x, T)) \sin(\alpha\pi) \Gamma(1 - \alpha) / \pi \quad \text{in } \Omega \quad (\text{terminal condition}), \\ f &= 0, q = 0 \quad \text{on } \Sigma \quad (\text{boundary conditions}), \\ v u + \left\langle \partial_x \left( \frac{\partial b}{\partial u} f \right), q \right\rangle &= 0 \quad \text{in } Q \quad (\text{optimality equations}), \end{aligned} \quad (15)$$

where we introduce the following inner product

$$\langle \phi, \psi \rangle = \int_0^T \int_{\Omega} \phi(x, t) \psi(x, t) (T - t)^{\alpha-1} dx dt.$$

Notice that the state variable evolves forward in time and the adjoint variable evolves backwards in time. Notice that the term  $(T - t)^{\alpha-1}$  in (12) enables to compute the terminal condition; see Appendix for the details of calculations. The operator  $\hat{\partial}_t^\alpha$  is an (almost) Erdélyi–Kober fractional operator, with the ordinary derivative inside the integral in the Caputo’s style. Furthermore, notice that assuming that  $f_d \in C_0^1(\bar{\Omega}) \cap C^2(\Omega)$ , then there exists a unique classical solution to the fractional adjoint equation.

We remark that the reduced gradient  $\nabla \hat{J}$  is given by the residue of the optimality equation as follows:

$$\nabla \hat{J} = v u + \left\langle \partial_x \left( \frac{\partial b}{\partial u} f \right), q \right\rangle, \quad (16)$$

where  $q = q(u)$  is the solution to the adjoint equation for the given  $f(u)$ .

### 3. DISCRETIZATION OF THE FFP OPTIMALITY SYSTEM

In this section, we discuss the numerical approximation to the forward and adjoint FFP equations using the CC [27] scheme for space discretization and the modified trapezoidal rule to approximate the Caputo time derivative. In [28], it is proved that the CC scheme is stable, second-order accurate,

positive, and conservative for FP equations with standard time derivatives. In particular, it is shown that positiveness and conservativeness depend on the CC spatial discretization, which is the same for the FFP equation written in the Caputo form.

The first step in the formulation of the CC scheme is to write the FFP equation in conservative flux form,  $\partial_t f = \nabla F$ . In fact, define the flux at  $(x, t)$  as follows:

$$F(x, t) = \frac{1}{2}a(x, t) \partial_x f(x, t) + \left( \frac{1}{2} \partial_x a(x, t) - b(x, t; u) \right) f(x, t).$$

Denote with

$$B(x, t, u) = \frac{1}{2} \partial_x a(x, t) - b(x, t; u)$$

and

$$C(x, t) = \frac{1}{2} a(x, t).$$

Therefore, we can write the FFP flux as follows:

$$F(x, t) = B(x, t) f(x, t) + C(x, t) \partial_x f(x, t), \tag{17}$$

and the FFP equation (6) becomes

$$\partial_t^\alpha f(x, t) = \partial_x F(x, t). \tag{18}$$

To illustrate the CC discretization, we consider a uniform mesh  $\Omega_h := \{x \in \mathbb{R} : x_i = ih, i \in \mathbb{Z}\} \cap \Omega$  of size  $h > 0$ , such that the boundaries of  $\Omega$  correspond to grid lines. We focus on the following semi-discretization of (18)

$$\partial_t^\alpha f_i(t) = \frac{1}{h} (F_{i+1/2}(t) - F_{i-1/2}(t)) \tag{19}$$

that involves the value of the fluxes at the boundaries of the cell  $i$ .

The CC scheme reconstructs the flux at the boundary  $i + 1/2$  of the cell  $i$  as follows:

$$F_{i+1/2} = \left[ (1 - \delta_i) B_{i+1/2} + \frac{1}{h} C_{i+1/2} \right] f_{i+1} - \left( \frac{1}{h} C_{i+1/2} - \delta_i B_{i+1/2} \right) f_i, \tag{20}$$

where  $\delta_i$  is a parameter specific of the CC scheme, given by

$$\delta_i = \frac{1}{w_i} - \frac{1}{\exp(w_i) - 1},$$

where  $w_i = h B_{i+1/2} / C_{i+1/2}$ , which can be shown to be monotonically decreasing from  $1/2$  to  $0$  as  $w_i$  goes from  $0$  to  $\infty$ . The CC reconstruction of flux at the boundary  $i - 1/2$  of the cell  $i$  proceeds similarly; see [19, 28] for more details.

Next, we discuss the discretization of the fractional time derivative of equation (7). We consider a time mesh with  $t_m = m\delta t$ ,  $m = 0, \dots, N$  on the interval  $[0, T]$ , with  $\delta t = T/N$ . We use the modified trapezoidal rule proposed in [40] to construct the approximation  $(D^\alpha f)(m)$  to  $(\partial_t^\alpha f)(t_m)$ . We have

$$(D^\alpha f)(m) = C \left( R_m f'_0 + \sum_{j=1}^{m-2} Q_{m,j} f'_j + (m \geq 2) c f'_{m-1} + f'_m \right),$$

where  $(m \geq 2)$  is a function of  $m$  defined as follows:  $(m \geq 2) = 1$  if  $m \geq 2$ , otherwise,  $(m \geq 2) = 0$  if  $m < 2$ . Further, we have

$$R_m = (m - 1)^{2-\alpha} - (m + \alpha - 2)m^{1-\alpha},$$

$$Q_{m,j} = (m - j + 1)^{2-\alpha} - 2(m - j)^{2-\alpha} + (m - j - 1)^{2-\alpha},$$

$C = \frac{\delta t^{-\alpha}}{2\Gamma(3-\alpha)}$ ,  $c = 2(2^{1-\alpha} - 1)$ ,  $f'_j$  is a difference operator approximation to  $f'(t_j)$ , and the summation is void for  $m \leq 2$ . Specifically, we construct second-order approximations to the derivatives as follows:  $f'_0 = (-3f_0 + 4f_1 - f_2)$ , the right difference;  $f'_j = (f_{j+1} - f_{j-1})$ ,  $j = 1, \dots, m - 1$ , the centred difference; and  $f'_m = (3f_m - 4f_{m-1} + f_{m-2})$ , the left difference.

For the case  $m = 2$ , we have

$$(D^\alpha f)(2) = C((3 + c - R_2)f_2 + H_1), \quad H_1 = (1 - c - 3R_2)f_0 - \alpha 2^{3-\alpha} f_1; \quad (21)$$

for  $m \geq 3$ , we have

$$(D^\alpha f)(m) = C((3 + c)f_m + H_{m-1}), \quad H_{m-1} = R_m f'_0 + \sum_{j=1}^{m-2} Q_{m,j} f'_j + (1 - c)f_{m-2} - 4f_{m-1}. \quad (22)$$

The value  $f_1$  can be calculated by using first-order difference approximation to  $f'_0$  and  $f'_1$ , with  $m = 1$ , so that

$$(D^\alpha f)(1) = 2C(1 + R_1)(f_1 - f_0), \quad R_1 = 1 - \alpha. \quad (23)$$

The starting value  $f_1$  can be calculated with better approximation by using more steps of a first-order approximation of the Caputo derivative.

The approximation of the Caputo adjoint operator (14)

$$-\hat{\partial}_t^\alpha q(x, t) = \frac{(T - t)^{-\alpha}}{\Gamma(1 - \alpha)} \int_t^T \left(\frac{T - s}{s - t}\right)^\alpha \partial_s q(x, s) ds \quad (24)$$

follows in a similar way. With the substitutions  $y = T - s$ ,  $g(y) = q(x, T - y)$ , and  $w = T - t$ , this operator becomes

$$\frac{w^{-\alpha}}{\Gamma(1 - \alpha)} \int_0^w \left(\frac{y}{w - y}\right)^\alpha g'(y) dy$$

so that the trapezoidal formula can be applied for discretization. As mentioned earlier, we distinguish the case  $m = 2$  from  $m \geq 3$ . Let  $w = m\delta t$ , then the three-points approximation formula is as follows:

$$m^{-\alpha} C (c(m - 1)^\alpha g'_{m-1} + m^\alpha g'_m).$$

We set  $T = N\delta t$ ,  $t_k = k\delta t$ ,  $m = N - k$ . Therefore, the case  $m = 2$  corresponds to  $k = N - 2$ , so that the previous expression reads as follows:

$$2^{-\alpha} C (c(N - k - 1)^\alpha g'_{N-1} + 2^\alpha q'_{N-2}).$$

Finally, we use the following difference operators

$$(\hat{D}^\alpha q)(2) = C(- (3 + 2^{-\alpha}c)q_{N-2} + \hat{H}_{N-1}), \quad \hat{H}_{N-1} = (2^{-\alpha}c - 1)q_N + 4q_{N-1} \quad (25)$$

to approximate (24) at  $t = T - 2\delta t$ .

Further, for the case  $m \geq 3$ , that is,  $k \leq N - 3$  ( $t \leq T - 3\delta t$ ), we have

$$\begin{aligned} (\hat{D}^\alpha q)(k) &= C\left(-\left(3 + c\left(\frac{N - k - 1}{N - k}\right)^\alpha\right)q_k + \hat{H}_{k+1}\right), \\ \hat{H}_{k+1} &= \sum_{l=k+2}^{N-1} Q_{l,k} \left(\frac{N - l}{N - k}\right)^\alpha q'_l + \left(c\left(\frac{N - k - 1}{N - k}\right)^\alpha - 1\right)q_{k+2} + 4q_{k+1}, \end{aligned} \quad (26)$$

where we use the equality  $Q_{N-k, N-l} = Q_{l,k}$ . Here,  $q_k$  is the unknown value that is calculated in a backward formula.

At last, we write a first-order formula for the evaluation of the second starting point

$$(\hat{D}^\alpha q)(1) = C(q_N - q_{N-1}). \tag{27}$$

With this preparation, we can write the discretized FFP equation with fractional Caputo time derivative as follows:

$$(3 + c)f_i^m + \frac{2\delta t^\alpha \Gamma(3 - \alpha)}{h} (F_{i+1/2}^m - F_{i-1/2}^m) = -H_{m-1}, \quad m \geq 3, \tag{28}$$

where  $f_i^m \approx f(x_i, t_m)$  and  $c = 2(2^{1-\alpha} - 1)$ . This formula needs three starting values,  $f^0$ ,  $f^1$ , and  $f^2$ , which are computed as follows:

$$f_i^1 + \frac{2\delta t^\alpha \Gamma(3 - \alpha)}{h(2 - \alpha)} (F_{i+1/2}^1 - F_{i-1/2}^1) = f_i^0,$$

and

$$(3 + c - R_2)f_i^2 + \frac{2\delta t^\alpha \Gamma(3 - \alpha)}{h} (F_{i+1/2}^2 - F_{i-1/2}^2) = -H_1,$$

where the initial condition is given by

$$f_i^0 = \rho(x_i). \tag{29}$$

For the discretization of the adjoint equation, we remark that the discrete space adjoint operator is obtained as the transpose of the corresponding operator in the forward equation. Further, we discretize the adjoint fractional time derivative as discussed earlier. We obtain the following discrete adjoint equation

$$\left(3 + c \left(\frac{N - m - 1}{N - m}\right)^\alpha\right) q_i^m + \frac{2\delta t^\alpha \Gamma(3 - \alpha)}{h} (F_{i+1/2}^m - F_{i-1/2}^m)^\top = \hat{H}_{m+1}, \quad m \leq N - 3. \tag{30}$$

This formula needs three starting values:  $q^{N_t}$ ,  $q^{N_t-1}$ , and  $q^{N_t-2}$ . The last two are calculated by using (27) and (25), respectively, as follows:

$$q_i^{N-1} + \frac{2\delta t^\alpha \Gamma(3 - \alpha)}{h} (F_{i+1/2}^{N-1} - F_{i-1/2}^{N-1})^\top = q_i^N,$$

and

$$(3 + 2^{-\alpha}c)q_i^{N-2} + \frac{2\delta t^\alpha \Gamma(3 - \alpha)}{h} (F_{i+1/2}^{N-2} - F_{i-1/2}^{N-2})^\top = \hat{H}_{N-1},$$

whereas  $q^N$  is given by the terminal condition

$$q_i^N = (f_d(x_i) - f_i^N) \sin(\alpha\pi) \Gamma(1 - \alpha)/\pi. \tag{31}$$

#### 4. A MODEL PREDICTIVE CONTROL SCHEME

Our purpose is to define a control strategy for the PDF of anomalous diffusion processes to track a given sequence of desired PDFs in time. In mathematical terms, this means to minimize the tracking objective (4) at given time instants. Let  $(0, T)$  be the time interval where the process is considered. We assume time windows of size  $\Delta t = T/K$  with  $K$  a positive integer, and  $t_k = k\Delta t$ ,  $k = 0, 1, \dots, K$ . On each time window  $(t_k, t_{k+1})$ , we consider an FFP optimal control as defined in (8)–(10), replacing 0 with  $t_k$  and  $T$  with  $t_{k+1}$ . At time  $t_0$ , we have a given initial PDF denoted with  $\rho$  and with  $f_d(\cdot, t_k)$ ,  $k = 1, \dots, K$ , we denote the sequence of desired PDFs. Our scheme starts at time  $t_0$  and solves the minimization problem  $\min_u J(f(u), u)$  defined in the interval  $(t_0, t_1)$ . Then, with the PDF  $f$  resulting at  $t = t_1$  that solves the optimal control problems (8)–(10) in  $(t_0, t_1)$ , we define the initial PDF for the subsequent optimization problem defined in the interval  $(t_1, t_2)$ . This procedure is repeated by receding the time horizon until the last time window is reached. This is an instance of the class of MPC schemes [25] that is widely used in engineering applications to



design closed-loop algorithms. One important aspect of this approach is that it can be applied to infinite dimensional evolution systems [41, 42] that are the case of the FFP model. Specifically, we implement an MPC scheme where the time horizon used to evaluate the control coincides with the time horizon where the control is used. We refer to [43] to show that the closed-loop system with the MPC scheme is nominally asymptotically stable.

The MPC procedure is summarized in the following algorithm.

*Algorithm 1 (MPC control)*

Set  $k = 0$ ,  $\rho_0 = \rho$ ;

- (1) Assign the initial PDF,  $f(x, t_k) = \rho_k(x)$ , and the target  $f_d(\cdot, t_{k+1})$ .
- (2) In  $(t_k, t_{k+1})$ , apply an NCG algorithm to solve  $\min_{u \in \mathbb{R}^{\ell}} J(f(u), u)$ , thus obtain the optimal pair  $(f, u)$ .
- (3) If  $t_{k+1} < T$ , set  $k := k + 1$ ,  $\rho_k = f(\cdot, t_k)$ , go to 1.
- (4) End.

Next, we discuss the second step of Algorithm 1, which consists in solving  $\min_u J(f(u), u)$  by a gradient-based method. To compute  $\nabla \hat{J}(u)$  for a given  $u$ , we have to solve first the forward FFP equation and then the adjoint FP equation. This procedure is summarized in the following algorithm.

*Algorithm 2 (Evaluation of the gradient at  $u$ )*

- (1) Solve the discrete FFP equation (28) with given initial condition (29).
- (2) Solve the discrete adjoint FFP equation (30) with terminal condition (31).
- (3) Compute the gradient  $\nabla \hat{J}(u)$  using (16).
- (4) End.

It is clear that the solution of the FFP optimality system may become prohibitive when high-dimensional anomalous stochastic processes are considered. In this case, special techniques for solving high-dimensional partial differential equations are in order; see, for example, [44, 45].

The reduced gradient computed by Algorithm 2 is the main input to an NCG scheme that we use; see [19, 46] for all details concerning our NCG implementation.

## 5. STOCHASTIC SIMULATION ALGORITHM

Our control strategy aims at determining a robust control function that is independent of the single realization of the anomalous diffusion process and nevertheless is able to drive all trajectories of the process to track a desired PDF target. In order to demonstrate this ability of our control framework, we plug our FFP control functions in the original stochastic process (1) and integrate the stochastic differential equations.

In this section, we describe the integration method of  $Y(t) = X(S(t))$ ,  $t \in [0, T]$ , that we use in our Monte Carlo simulation. The method consists of three steps; see [10, 21] for additional details.

In the first step, we approximate  $S(t)$  using the following approximation scheme:

$$S_{\delta}(t) = (\min\{n \in \mathbb{N} : U(\delta n) > t\} - 1) \delta,$$

where  $\delta > 0$  is the accuracy parameter, that is, the integration step. Recall that  $U(t)$  is the strictly increasing  $\alpha$ -stable Lévy motion. Thus, the values  $U(\delta n)$  in the aforementioned formula can be obtained using the following Euler scheme [47]:

$$\begin{aligned} U(0) &= 0, \\ U(\delta n) &= U(\delta(n-1)) + \delta^{1/\alpha} \xi_n, \end{aligned}$$

where  $\xi$ , for any step  $n \in \mathbb{N}$ , are the i.i.d. totally skewed positive  $\alpha$ -stable random variables. The procedure of generating realizations of  $\xi$  is described by the following formula:

$$\xi = \frac{\sin(\alpha(V + c_1))}{(\cos(V))^{1/\alpha}} \left( \frac{\cos(V - \alpha(V + c_1))}{W} \right)^{(1-\alpha)/\alpha},$$

where  $c_1 = \pi/2$ , the random variable  $V$  is uniformly distributed on  $(-\pi/2, \pi/2)$ , and  $W$  has exponential distribution with mean one.

In the second step, we integrate the process  $X(t)$  using the classical Euler scheme

$$\begin{aligned} X(0) &= 0, \\ X(\delta n) &= X(\delta(n-1)) + b(X(\delta(n-1)); u)\delta + \delta^{1/2}\sigma(X(\delta(n-1)))\zeta_n. \end{aligned} \quad (32)$$

Here,  $\zeta_n, n \in \mathbb{N}$ , are the i.i.d. standard normal random variables.

Finally, in the third step, we compose  $X$  with  $S_\delta$  obtained in the previous step, to obtain one approximated trajectory of  $Y(t) = X(S(t))$ .

## 6. APPLICATIONS

In this section, we discuss the optimal control of the PDF of a fractional OU process. In particular, we show the ability of our control strategy for our FFP model to track a desired trajectory configuration and present results of a Monte Carlo simulation to demonstrate that the same control is able to drive the trajectories of the OU anomalous diffusion stochastic process accordingly to the desired target PDFs.

The fractional OU process has important applications in numerous areas such as physics [11, 13, 48] and finance [49–51]. In this model, the drift term is given by  $b(x, u) = -\gamma x + u$ . In our experiments, we choose  $\gamma = 0.1$ ,  $a = 0.16$ , and fractional diffusion  $\alpha = 0.6$ . The initial PDF  $\rho(x)$  is given by a Gaussian normal density placed in 0 with variance  $\sigma = 0.1$ . The target function in (4) is a Gaussian density with  $\sigma = \sqrt{0.4}$  and mean that is stepwise constant in time according to the setting  $\mu(t) = \mu_k I_{\tau_k, \tau_{k+1}}(t)$ ,  $\mu = \{0.6, 0.2, -1, 0.4\}$ , and  $\tau = \{0, 0.2, 0.5, 0.7, 1\}$ . The weight of the cost of the control is  $\nu = 0.05$ . The aim is to control the PDF evolution to the final time  $T = 1$  using 10 MPC time windows of size  $\Delta t = 0.1$ . For the numerical calculation, we discretized the space domain  $[-L, L]$ ,  $L = 10$  with  $N_x = 400$  points and the time domains  $[t_k, t_{k+1}]$  with  $N_t = 200$  points. In Figure 1, we see results of numerical experiments with  $\alpha = 0.6$ , where we plot the target and the controlled PDF for each MPC time window. We can see that the controlled PDF follows the target. In Figure 2, we depict the calculated piecewise control  $u$  (dashed line), and the corresponding maximum norm of the tracking error, that is, the difference between the target PDF and the controlled PDFs.

Next, we test the ability of our FFP control function to drive the trajectories of the fractional OU stochastic process. For this purpose, we perform Monte Carlo tests where the stochastic trajectories are computed with the integration method described in Section 5.

Consider a Monte Carlo simulation where the values of the control  $u$  are those depicted in Figure 2. The numerical integration of a single trajectory starts at time  $t = t_0$  with  $u = u_0$  and stops at  $t = t_1$ . The final value  $X_{t_1}$  is then used as the initial condition for the following time window  $[t_1, t_2]$ , where the control is updated to  $u = u_1$ . The integration proceeds in this way up to the last time window. Then the integration process is restarted and repeated 500 times. In Figure 3, the first 10 trajectories are plotted. In the same figure in the succeeding text, we plot the corresponding values of the controls for each time window. The pictures on the right-hand side show the histograms collecting the final positions of the process. For ease of visualization, we report, on the top figures, the trajectories and the corresponding histogram for 10 trajectories. The histograms of a complete test are plotted in the bottom right figure, together with the calculated PDF and the target at the final time. We see that the distribution of the final histograms of the positions of the process is in very good agreement with the PDF resulting from the FFP model.

## 7. CONCLUSION

The formulation of an FFP framework for determining controls of subdiffusion processes with objectives formulated with the PDF of the processes was presented. The control strategy was based on an MPC scheme consisting of a sequence of open-loop FFP optimal control problems with PDF

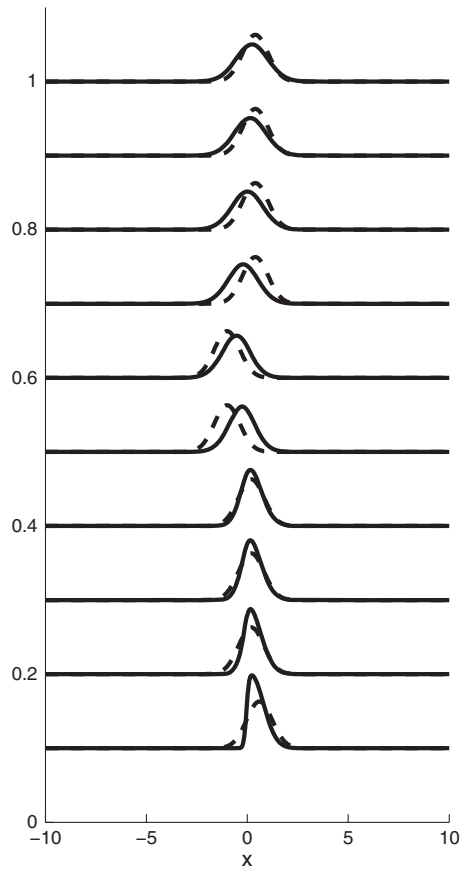


Figure 1. Control sequence over 10 MPC time windows of size 0.1, for the OU FFP model with  $\alpha = 0.6$ . Dashed line: target; solid line: controlled PDFs.

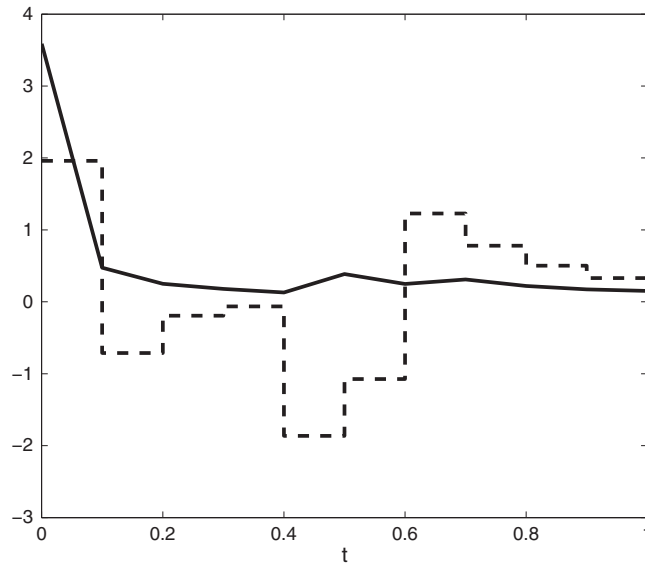


Figure 2. Evolution in time of the tracking error (solid) and the corresponding piecewise control (dashed);  $\alpha = 0.6$ .

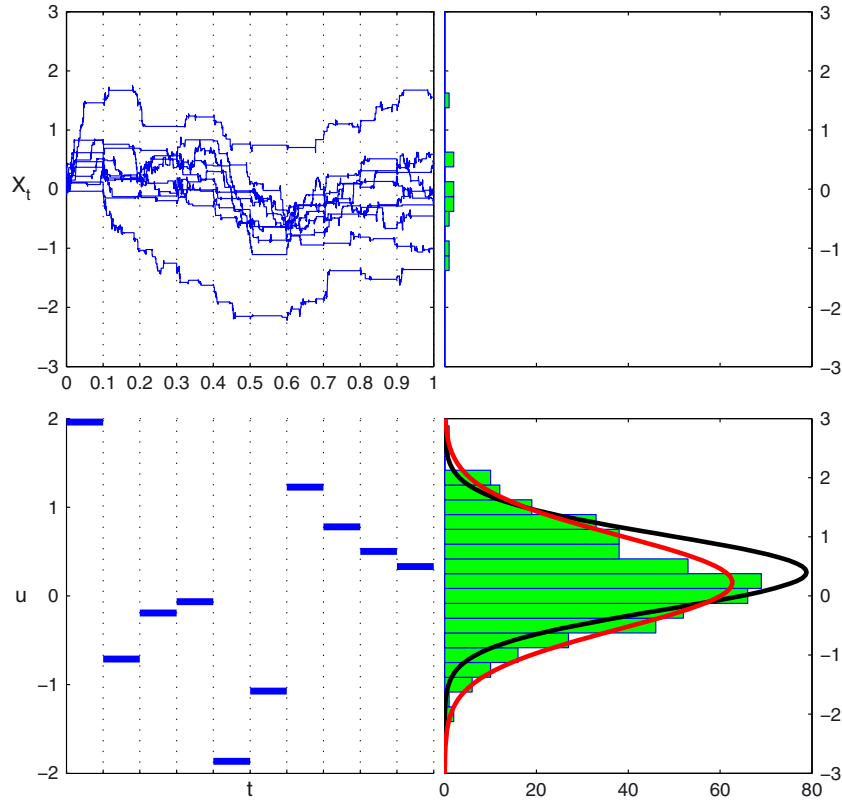


Figure 3. Monte Carlo test. Ten samples of the optimally controlled trajectories for the fractional OU process with  $\alpha = 0.6$  (upper left); values of the piecewise control over the time windows (bottom left); histograms of the first 10 samples (upper right); histograms of 500 samples, the scaled controlled PDF (red/grey), and the PDF target (black) (bottom right).

tracking objectives. To solve these optimal control problems, the corresponding FFP optimality system was derived and discretized by an accurate and positivity preserving scheme, and the resulting gradient was used to implement an NCG strategy. The effectiveness of the proposed FFP control framework was validated with numerical experiments involving the solution of the FFP model and simulation of the corresponding subdiffusion process.

The results presented in this paper open a new direction of further research inspired by competition between subdiffusion and jump diffusion (e.g., Lévy flights); see [30, 52, 53].

#### APPENDIX A: THE ADJOINT TIME DERIVATIVE

In this appendix, we discuss the derivation of the adjoint time derivative and of the terminal condition in the fractional optimality system. For this purpose, we consider the part of the Lagrangian (12) that involves time derivatives. We have

$$\int_{\Omega} \int_0^T \partial_t^\alpha f(x, t) q(x, t) (T - t)^{\alpha-1} dx dt.$$

Including the variation and taking the limit, we obtain the following:

$$\frac{1}{\Gamma(1 - \alpha)} \int_{\Omega} \int_0^T \int_s^T \frac{\partial_s \delta f(x, s)}{(t - s)^\alpha} q(x, t) (T - t)^{\alpha-1} dt ds dx;$$

that is,

$$\frac{1}{\Gamma(1 - \alpha)} \int_{\Omega} \int_0^T \partial_t \delta f(x, t) \int_t^T \frac{q(x, s) (T - s)^{\alpha-1}}{(s - t)^\alpha} ds dt dx$$

and integrating by parts

$$\frac{1}{\Gamma(1-\alpha)} \int_{\Omega} \left[ \left( \delta f(x, t) \int_t^T \frac{q(x, s)(T-s)^{\alpha-1}}{(s-t)^{\alpha}} ds \right) \Big|_0^T - \int_0^T \delta f(x, t) \partial_t \left( \int_t^T \frac{q(x, s)(T-s)^{\alpha-1}}{(s-t)^{\alpha}} ds \right) dt \right] dx.$$

Note that  $\lim_{t \rightarrow T} \int_t^T \frac{q(x, s)(T-s)^{\alpha-1}}{(s-t)^{\alpha}} ds = \pi q(x, T) / \sin(\alpha\pi)$ . This result can be obtained extracting  $q(x, s)$  from the integral, by the first mean value theorem for integration. The integral is calculated with formula 3.191.2 of [54], then the limit gives the result. Thus, we obtain

$$\frac{1}{\Gamma(1-\alpha)} \int_{\Omega} \left[ \pi \delta f(x, T) q(x, T) / \sin(\alpha\pi) - \delta f(x, 0) \int_0^T \frac{q(x, s)(T-s)^{\alpha-1}}{s^{\alpha}} ds - \int_0^T \delta f(x, t) \partial_t \left( \int_t^T \frac{q(x, s)(T-s)^{\alpha-1}}{(s-t)^{\alpha}} ds \right) dt \right] dx. \tag{A.1}$$

Because of the initial condition, we have  $\delta f(x, 0) = 0$ . Including the variation of the cost functional (4), we collect the following terms

$$\int_{\Omega} \left[ f(x, T) - f_d(x) + \frac{\pi q(x, T)}{\sin(\alpha\pi)\Gamma(1-\alpha)} \right] \delta f(x, T) dx,$$

because  $\delta f(x, T) \neq 0$ , the terminal condition reads as follows

$$q(x, T) = (f_d(x) - f(x, T)) \sin(\alpha\pi)\Gamma(1-\alpha)/\pi.$$

From the last integral of (A.1), we obtain the adjoint time operator, that is, a Riemann fractional integral. This integral can be recast to the Caputo form as follows. Let  $Q(s, t) = \int (T-s)^{\alpha-1} / (s-t)^{\alpha} ds = -(T-s)^{\alpha} / (s-t)^{\alpha} {}_2F_1(\alpha, \alpha, 1+\alpha, (T-s)/(T-t)) / \alpha$ , for  $t \leq s \leq T$ , where  ${}_2F_1$  is an hypergeometric function. It is  $Q(t, t) = -\pi / \sin(\alpha\pi)$ ,  $Q(T, t) = 0$ . Integrating by parts the integral in  $ds$ ,

$$\partial_t \left[ q(x, t) \pi / \sin(\alpha\pi) - \int_t^T \partial_s q(x, s) Q(s, t) ds \right] = - \int_t^T \partial_s q(x, s) \partial_t Q(s, t) ds,$$

and thus, the adjoint operator of (14) is obtained.

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