

# Source terms identification for time fractional diffusion equation

Identificación de términos fuente en ecuaciones de difusión en las que la derivada con respecto al tiempo es fraccional

DIEGO A. MURIO<sup>1,a</sup>, CARLOS E. MEJÍA<sup>2,b</sup>

<sup>1</sup>University of Cincinnati, Ohio, USA

<sup>2</sup>Universidad Nacional de Colombia, Medellín, Colombia

**ABSTRACT.** We introduce a regularization technique for the approximate reconstruction of spatial and time varying source terms using the observed solutions of the forward time fractional diffusion problem on a discrete set of points. The numerical method is based on computation of the derivatives of adaptive filtered versions of the noisy data by *discrete mollification*.

**Key words and phrases.** Ill-Posed Problems, heat source identification, Caputo fractional derivatives, time fractional diffusion equation, mollification techniques.

**2000 Mathematics Subject Classification.** 65M06, 65M12, 65M30, 65M32.

**RESUMEN.** Presentamos una técnica de regularización para la reconstrucción numérica de términos fuente dependientes de espacio y tiempo a partir de aproximaciones de la solución del problema directo en un conjunto discreto de puntos. El método se basa en el cálculo de derivadas de versiones de los datos aproximados que se obtienen con el filtro adaptativo denominado *mollificación discreta*.

**Palabras y frases clave.** Problemas mal condicionados, identificación de una fuente de calor, derivadas fraccionales de Caputo, ecuación de difusión con derivada fraccional en la dirección del tiempo, técnicas de mollificación.

---

<sup>a</sup>Partial support from a C. P. Taft Fellowship.

<sup>b</sup>Partial support from Universidad Complutense de Madrid, España and Universidad Nacional de Colombia, DIME project number 30802867.

## 1. Introduction

We consider a family of time fractional diffusion equations of the form

$$D_t^{(\alpha)} u(x, t) = a(x, t) \frac{\partial^2 u(x, t)}{\partial x^2} + f(x, t), \quad 0 < x < 1, \quad 0 < t < 1, \quad (1)$$

together with the corresponding boundary and initial conditions

$$\begin{aligned} u(0, t) &= u_0(t), \quad 0 \leq t \leq 1, \\ u(1, t) &= u_1(t), \quad 0 \leq t \leq 1, \\ u(x, 0) &= u^0(x), \quad 0 \leq x \leq 1, \end{aligned}$$

where the symbol  $D_t^{(\alpha)}$  denotes Caputo's partial fractional derivative of order  $\alpha$  with respect to time,  $0 < \alpha \leq 1$ .

Ordinarily,  $f(x, t)$  and  $a(x, t)$  are known functions and we are asked to determine the solution function  $u(x, t)$  so as to satisfy equation (1) and the boundary and initial conditions. So posed, this is a direct problem.

There are, however, several interesting inverse problems that can be formulated. Our main objective in this work is to determine part of the structure of the system, in our case the forcing term  $f$ , from experimental information given by the approximate knowledge of the function  $u$  at a discrete set of points in its domain. This question belongs to a general class of inverse problems, known as system identification problems, and, in particular, it is an ill-posed problem because small errors in the function  $u$  might cause large errors in the computation of the derivatives  $D_t^{(\alpha)} u$  and  $\frac{\partial^2 u}{\partial x^2}$  which are needed in order to estimate the forcing term function  $f$ .

To better illustrate the poor stability properties of the mapping from the data function  $u$  to the solution function  $f$ , let us consider a semi-infinite vertical slab in the  $(x, t)$  plane, where the temperature function  $u$  satisfies a classical heat equation, corresponding in our terminology to the case  $\alpha = 1$ ,

$$D_t^{(1)} u = \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + f(x, t), \quad 0 < x < \pi, \quad 0 < t < \infty,$$

with homogeneous (zero) boundary and initial conditions. We wish to reconstruct  $f(x, t)$  from the *exact* transient temperature history  $T(t) = u(x_0, t)$  given at some point  $x_0$ ,  $0 < x_0 < \pi$ . Separation of variables leads to the integral representation

$$T(t) = \int_0^t \int_0^\pi k(x, t-s) f(x, s) dx ds,$$

where the kernel function is given by

$$k(x, \tau) = \frac{2}{\pi} \sum_{n=1}^{\infty} e^{-n^2 \tau} \sin(nx_0) \sin(nx).$$

Introducing the sequence of data functions

$$T_n(t) = n^{-3/2} \left( 2 - e^{-n^2 t} \right) \sin(nx_0), \quad n = 0, 1, 2, \dots,$$

the source terms  $f_n$  are independent of  $t$  and we obtain

$$f_n(x) = 2\sqrt{n} \sin(nx).$$

From here, it is clear that when  $T_n \rightarrow 0$ ,  $\max_{0 < x < \pi} |f_n(x)| = 2\sqrt{n} \rightarrow \infty$  as  $n \rightarrow \infty$ , showing that the problem is greatly ill-posed with respect to perturbations in the data.

The identification of parameters in classical parabolic equations ( $\alpha = 1$ ) is an ill-posed problem that has received considerable attention from many researchers in a variety of fields, using different methods. Some detailed treatments of problems in these areas can be found in [5] and [30]. The use of space marching schemes along with the methods of discrete mollification-implemented as an automatic iterative filtering- and generalized cross validation (GCV), has proven to be an effective way for solving these problems [8], [10], [12], [18]. For an up to date detailed description of these techniques see the chapter on mollification in the *Inverse Engineering Handbook* [20].

In particular, the determination of source terms in the one-dimensional ( $\alpha = 1$ ) inverse heat conduction problem (IHCP) is a parameter identification type of problem that has been extensively explored. The available results are based on the assumptions that the source term depends only on one variable [3] or that it can be separated into spatial and temporal components [8], [11], [25].

If the temperature distribution is known approximately on the entire domain of interest, the successful reconstruction of general source terms for the case  $\alpha = 1$  is described in [31]. In this paper we extend the results presented in [31] to transport processes with long memory where the rate of diffusion is inconsistent with the classical Brownian motion model ( $0 < \alpha < 1$ ).

The manuscript is organized as follows: in section 2, for completeness, we state basic properties and estimates associated with mollification and fractional derivatives and introduce the fractional diffusion equations. Section 3 is devoted to the description of the stabilized identification problem and the corresponding error analysis of the approximate solution. In section 4 we briefly describe a fully implicit unconditionally stable numerical method needed to generate the data for the inverse problem when modeling. To illustrate the efficiency of the proposed identification approach, several numerical examples of interest are also presented and analyzed in this section.

## 2. Preliminaries

**2.1. Mollification.** Let  $C^0(I_t)$  denote the set of continuous real functions over the unit interval  $I_t = [0, 1]$  with norm

$$\|g\|_{\infty, I_t} = \max_{t \in I_t} |g(t)|,$$

and introduce the kernel function

$$\rho_{\delta,p}(t) = \begin{cases} A_p \delta^{-1} \exp\left(-\frac{t^2}{\delta^2}\right), & |t| \leq p\delta, \\ 0, & |t| > p\delta, \end{cases} \quad (2)$$

where  $\delta > 0$ ,  $p > 0$ , and  $A_p = \left(\int_{-p}^p \exp(-s^2) ds\right)^{-1}$ . The  $\delta$ -mollifier  $\rho_{\delta,p}$  is a non-negative  $C^\infty(-p\delta, p\delta)$  function satisfying  $\int_{-p\delta}^{p\delta} \rho_{\delta,p}(x) dx = 1$ .

For  $g \in L^1(I_t)$  and for  $t \in I_t^\delta = [p\delta, 1 - p\delta]$  the  $\delta$ -mollification of  $g$  is defined by the convolution

$$\begin{aligned} J_\delta g(t) &= (\rho_\delta * g)(t) = \int_{I_t^\delta} \rho_\delta(t-s)g(s)ds \\ &= \int_{t-p\delta}^{t+p\delta} \rho_\delta(t-s)g(s)ds, \end{aligned}$$

where the  $p$ -dependency on the kernel has been dropped for simplicity of notation. We observe that  $p\delta = \text{dist}(I_t, \partial I_t^\delta)$ .

The following three lemmas are needed for the stability analysis of the source terms reconstruction in section 3. The proofs can be found in [20], [19], [24].

We assume that instead of the function  $g$ , we know some noisy data function  $g^\epsilon \in C^0(I_t)$  such that  $\|g - g^\epsilon\|_{\infty, I_t} \leq \epsilon$ .

In all cases, the discrete (sampled) functions  $G = \{g(t_j) : j \in Z\}$  and  $G^\epsilon = \{g^\epsilon(t_j) : j \in Z\}$  are defined on a uniform partition  $K_t$  of  $I_t$ , with step size  $\Delta t$ , and satisfy  $\|G - G^\epsilon\|_{\infty, I_t \cap K_t} \leq \epsilon$ . The symbol  $C$  represents a generic positive real constant.

**Lemma 1.** *If  $g \in C^0(I_t)$  then there exists a constant  $C$ , independent of  $\delta$ , such that  $\|J_\delta G^\epsilon - J_\delta g\|_{\infty, I_t^\delta \cap K_t} \leq C(\epsilon + \Delta t)$  and  $\|J_\delta G^\epsilon - g\|_{\infty, I_t^\delta \cap K_t} \leq C(\epsilon + \delta + \Delta t)$ .*

**Lemma 2.** *If  $\frac{dg}{dt} \in C^0(I_t)$ , then there exists a constant  $C$ , independent of  $\delta$ , such that*

$$\left\| \frac{d}{dt} J_\delta G^\epsilon - \frac{d}{dt} g \right\|_{\infty, I_t^\delta \cap K_t} \leq C \left( \delta + \frac{\epsilon + \Delta t}{\delta} \right).$$

Moreover, if  $\frac{d^2 g}{dt^2} \in C^0(I_t)$ , then

$$\left\| \frac{d^2}{dt^2} J_\delta G^\epsilon - \frac{d^2}{dt^2} g \right\|_{\infty, I_t^\delta \cap K_t} \leq C \left( \delta + \frac{\epsilon + \Delta t}{\delta^2} \right).$$

**Lemma 3.** *If  $g \in C^0(I_t)$ , then there exists a constant  $C$ , independent of  $\delta$ , and a constant  $C_\delta$ , independent of  $\Delta t$ , such that*

$$\left\| D_0(J_\delta G^\epsilon) - \frac{d}{dt} g \right\|_{\infty, I_t^\delta \cap K_t} \leq C \left( \delta + \frac{\epsilon + \Delta t}{\delta} \right) + C_\delta (\Delta t)^2$$

and

$$\left\| D_+ D_- (J_\delta G^\epsilon) - \frac{d^2}{dt^2} g \right\|_{\infty, I_t^\delta \cap K_t} \leq C \left( \delta + \frac{\epsilon + \Delta t}{\delta^2} \right) + C_\delta (\Delta t)^2,$$

where  $D_0$  and  $D_+ D_-$  denote the centered and backward-forward finite difference approximations to the first and second derivatives, respectively.

These lemmas demonstrate that attempting to reconstruct mollified derivatives from noisy data functions, in a suitable subset of their domains, is a stable problem with respect to perturbations in the data, in the maximum norm. When discrete mollification is taken as a finite dimensional linear operator, the estimates are different but similar and can be found, for instance, in [1].

To get formal convergence, the ill-posedness of the problem requires to relate all the parameters involved. The choice  $\delta = (\epsilon + \Delta t)^{1/3}$  shows that, for example,

$$\left\| \frac{d^2}{dt^2} J_\delta G^\epsilon - \frac{d^2}{dt^2} g \right\|_{\infty, I_t^\delta \cap K_t} = O(\epsilon + \Delta t)^{1/3},$$

which implies formal convergence as  $\epsilon$  and  $\Delta t \rightarrow 0$ .

**2.2. Fractional derivatives.** The usual formulation of the fractional derivative, given in standard references such as [26], [27] and [28], is the Riemann-Liouville definition.

The Riemann-Liouville fractional derivative of order  $\alpha$ , ( $0 < \alpha \leq 1$ ) of an integrable function  $g$  defined on  $I_t$ , is defined by the integro-differential operator

$$\begin{aligned} ({}_0 D^{(\alpha)} g)(t) &= \frac{1}{\Gamma(1-\alpha)} \frac{d}{dt} \int_0^t \frac{g(s)}{(t-s)^\alpha} ds, & 0 \leq t \leq 1, & \quad 0 < \alpha < 1, \\ ({}_0 D^{(\alpha)} g)(t) &= \frac{dg(t)}{dt}, & 0 \leq t \leq 1, & \quad \alpha = 1, \end{aligned}$$

where  $\Gamma(\cdot)$  is the Gamma function.

This definition leads to fractional differential equations which require the initial conditions to be expressed not in terms of the solution itself but rather in terms of its fractional derivatives, which are difficult to derive from a physical system. In applications it is often more convenient to use the formulation of the fractional derivative suggested by Caputo [4] which requires the same starting condition as an ordinary differential equation of order 1.

The Caputo fractional derivative of order  $\alpha > 0$ , of a differentiable function  $g$  defined on  $I_t$ , is given by the integro-differential operator

$$\begin{aligned} (D^{(\alpha)} g)(t) &= \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{g'(s)}{(t-s)^\alpha} ds, & 0 \leq t \leq 1, & \quad 0 < \alpha < 1, \\ (D^{(\alpha)} g)(t) &= \frac{dg(t)}{dt}, & 0 \leq t \leq 1, & \quad \alpha = 1. \end{aligned} \quad (3)$$

The integral part of this fractional differential operator is a convolution integral with weakly singular kernel and the above formulation is of little use in practice unless the data is known exactly.

In the presence of noisy data  $g^\epsilon$ , instead of recovering  $D^{(\alpha)}g$ , we look for a mollified solution  $J_\delta(D^{(\alpha)}g^\epsilon)$  obtained from the previous equation by convolution with the normalized Gaussian kernel  $\rho_\delta$ .

Consequently, instead of equation (3) we have

$$J_\delta(D^{(\alpha)}g^\epsilon)(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{(J_\delta g^\epsilon)'(s)}{(t-s)^\alpha} ds. \quad (4)$$

It is shown in [21] that the mollified formula (4) satisfies the following error estimate.

**Theorem 4.** *If the functions  $g'$  and  $g^\epsilon$  are uniformly Lipschitz on  $I_t$  and  $\|g - g^\epsilon\|_{\infty, I_t} \leq \epsilon$ , then there exists a constant  $C$ , independent of  $\delta$ , such that*

$$\|J_\delta(D^{(\alpha)}g^\epsilon) - D^{(\alpha)}g\|_{\infty, I_t} \leq \frac{C}{(1-\alpha)\Gamma(1-\alpha)} \left( \delta + \frac{\epsilon}{\delta} \right).$$

Stability is valid for each fixed  $\delta > 0$  and the optimal rate of convergence is obtained by choosing  $\delta = O(\sqrt{\epsilon})$ .

The mollified Caputo fractional derivative, reconstructed from noisy data, tends uniformly to the exact solution as  $\epsilon \rightarrow 0$ ,  $\delta = \delta(\epsilon) \rightarrow 0$ . This establishes the consistency, stability and formal convergence properties of the procedure.

**Remark 5.** *The mollified formula (4) necessitates the extension of the data function to the interval  $(-p\delta, 1+p\delta)$  to evaluate  $J_\delta(D^{(\alpha)}g^\epsilon)$  for every  $t$  in  $I_t$  (see [21], [33] and the references therein) since the evaluation of  $J_\delta(D^{(\alpha)}g^\epsilon)(t)$  requires the knowledge of the fractional derivative at all the previous grid points in time.*

**2.3. Numerical Implementation.** To numerically approximate  $J_\delta(D^{(\alpha)}g)$ , the following quadrature formula for the convolution equation (4), on a uniform partition  $K_t$  of the unit interval  $I_t$ , was implemented in [21].

The discrete computed solution, denoted  $(D^{(\alpha)}G^\epsilon)_\delta$ , when restricted to the grid points, gives

$$\begin{aligned} (D^{(\alpha)}G^\epsilon)_\delta(t_1) &= D_+(J_\delta G^\epsilon)(t_1)W_1, \\ (D^{(\alpha)}G^\epsilon)_\delta(t_2) &= D_+(J_\delta G^\epsilon)(t_1)W_1 + D_+(J_\delta G^\epsilon)(t_2)W_2, \\ (D^{(\alpha)}G^\epsilon)_\delta(t_j) &= D_+(J_\delta G^\epsilon)(t_1)W_1 + \sum_{i=2}^{j-1} D_0(J_\delta G^\epsilon)(t_i)W_{j-i+1} \\ &\quad + D_+(J_\delta G^\epsilon)(t_j)W_j, \quad j = 3, \dots, n. \end{aligned} \quad (5)$$

Here the quadrature weights  $W_j = W_j(\alpha, \Delta t)$  are integrated exactly with values

$$W_1 = \frac{1}{\Gamma(1-\alpha)} \frac{1}{1-\alpha} \left( \frac{\Delta t}{2} \right)^{1-\alpha},$$

$$W_i = \frac{1}{\Gamma(1-\alpha)} \frac{1}{1-\alpha} \left[ \left( (2i+1) \frac{\Delta t}{2} \right)^{1-\alpha} - \left( (2i-1) \frac{\Delta t}{2} \right)^{1-\alpha} \right],$$

$$i = 2, \dots, j-1$$

and

$$W_j = \frac{1}{\Gamma(1-\alpha)} \frac{1}{1-\alpha} \left[ j\Delta t - \left[ \left( j - \frac{1}{2} \right) \Delta t \right]^{1-\alpha} \right].$$

The quadrature formula satisfies the following error estimate.

**Theorem 6.** *If the functions  $g'$  and  $g^\epsilon$  are uniformly Lipschitz on  $I_t$  and  $G$  and  $G^\epsilon$ , the discrete versions of  $g$  and  $g^\epsilon$  respectively, satisfy  $\|G - G^\epsilon\|_{\infty, I_t \cap K_t} \leq \epsilon$ , then:*

$$\left\| \left( D^{(\alpha)} G^\epsilon \right)_\delta - D^{(\alpha)} g \right\|_{\infty, I_t^\delta \cap K_t} \leq \frac{C}{\Gamma(1-\alpha)(1-\alpha)} \left( \delta + \frac{\epsilon}{\delta} + \Delta t \right).$$

The error estimate for the discrete case is obtained by adding the global truncation error to the error estimate of the non-discrete case.

**Remark 7.** *The time fractional derivative  $(D^{(\alpha)} G^\epsilon)_\delta$  is computed initially on the entire discrete set  $I_t \cap K_t$  (Remark 5), and then restricted to  $I_t^\delta \cap K_t$ .*

**2.4. Fractional diffusion equations (FDE).** We start with some definitions: the diffusion process is called *subdiffusion* if  $0 < \alpha < 1$  and *superdiffusion* if  $1 < \alpha \leq 2$ . If the partial fractional derivative is applied to the time variable, the FDE is called *time fractional diffusion equation* (TFDE). The study of fractional diffusion equations is receiving a lot of attention recently as can be seen, for instance, in [2], [6], [14], [15], [17].

**2.4.1. Linear time fractional diffusion equation.** We are interested solely on time fractional diffusion equations (TFDE) and in this case there are two common formulations depending on the type of time fractional derivative employed and its location in the partial differential equation.

Using Caputo fractional derivatives, a natural extension of the standard formulation of the diffusion equation corresponding to  $\alpha = 1$ , the TFDE is

described by

$$\begin{aligned} D_t^{(\alpha)} u(x, t) &= \frac{\partial^2 u(x, t)}{\partial x^2} + f(x, t), \quad 0 < x < 1, \quad t > 0, \\ u(0, t) &= u_0(t), \quad t \geq 0, \\ u(1, t) &= u_1(t), \quad t \geq 0, \\ u(x, 0) &= u^0(x), \quad 0 \leq x \leq 1. \end{aligned} \quad (6)$$

Another fractional diffusion equations, using Grünwald-Letnikov fractional derivatives [23], [32] or Riemann-Liouville fractional derivatives [13], are obtained by writing the governing equation as

$$\frac{\partial u(x, t)}{\partial t} = {}_w D_t^{(1-\alpha)} \left( \frac{\partial^2 u(x, t)}{\partial x^2} \right) + f(x, t), \quad 0 < x < 1, \quad t > 0 \quad (7)$$

where  $w$  is 1 for Grünwald-Letnikov and 0 for Riemann-Liouville fractional derivatives respectively.

In this paper we work only with forcing terms identification in the TFDE version described by the system (6). For other approaches to FDE and a review of numerical methods we recommend [7], [9] and [16]. On implicit schemes for the approximation of fractional derivatives there are several recent papers, for instance [22], [34] and [35]. An explicit conservative scheme can be found in [29].

### 3. Stabilized source problem

We consider the temperature function  $u(x, t)$  measured in the unit square  $I = I_x \times I_t = [0, 1] \times [0, 1]$  of the  $(x, t)$  plane. On the basis of this information we discuss the problem of estimating the forcing term function  $f$  in some suitable compact set  $Q \subseteq I$ . We assume the functions  $u$ ,  $a$ ,  $u_{xx}$  and  $f$  are in  $C^0(I)$  and that instead of the function  $u$ , we know some data function  $u^\epsilon \in C^0(I)$  so that  $\|u - u^\epsilon\|_{\infty, I} \leq \epsilon$ .

If  $K_x$  and  $K_t$  denote uniform partitions of  $I_x$  and  $I_t$ , with step sizes  $\Delta x$  and  $\Delta t$  respectively, the discrete data temperature is measured at the grid points  $K_x \times K_t \subseteq I$  and the source terms are reconstructed on the discrete set of points  $K = (K_x \times K_t) \cap Q$ .

The regained stability properties established in the previous section are naturally inherited by the mollified reconstructed source term which is obtained as a linear combination of mollified partial derivatives of the measured temperature function. More precisely, if  $(x_i, t_n) \in K$ , we have

$$J_\delta f^\epsilon(x_i, t_n) = \left( D_t^{(\alpha)} u^\epsilon(x_i, t_n) \right)_\delta - a(x_i, t_n) D_+ D_- (J_\delta u^\epsilon(x_i, t_n)). \quad (8)$$

We can now state our main theoretical result.

**Theorem 8.** *Under the conditions of lemma 3 and theorem 6, for fixed  $\delta > 0$ , the reconstructed mollified source term  $J_\delta f^\epsilon$  given by formula (8), satisfies*

$$\|J_\delta f^\epsilon - f\|_{\infty, K} \leq C \left\{ \delta + \frac{\epsilon + \Delta t + \Delta x}{\delta^2} \right\} + C_\delta \{(\Delta x)^2 + (\Delta t)^2\}.$$

*Proof.* Restricting equations (1) and (8) to the grid points, rearranging terms, subtracting, and using maximum norms, we have

$$\begin{aligned} \|J_\delta f^\epsilon - f\|_{\infty, K} &\leq \|a\|_{\infty, K} \left\| D_+ D_- (J_\delta u^\epsilon) - \frac{\partial^2 u}{\partial x^2} \right\|_{\infty, K} \\ &\quad + \left\| \left( D_t^{(\alpha)} u^\epsilon \right)_\delta - \left( D_t^{(\alpha)} u \right) \right\|_{\infty, K}. \end{aligned}$$

Applying lemma 3 and theorem 6 to the last expression,

$$\begin{aligned} \|J_\delta f^\epsilon - f\|_{\infty, K} &\leq \|a\|_{\infty, K} \left\{ C \left( \delta + \frac{\epsilon + \Delta x}{\delta^2} \right) + C_\delta (\Delta x)^2 \right\} \\ &\quad + \frac{C}{\Gamma(1-\alpha)(1-\alpha)} \left( \delta + \frac{\epsilon}{\delta} + \Delta t \right). \end{aligned}$$

Setting  $M = \max \|a\|_{\infty, I}$ , we obtain the final estimate

$$\|J_\delta f^\epsilon - f\|_{\infty, K} \leq CM \left\{ \delta + \frac{\epsilon + \Delta x}{\delta^2} + \Delta t \right\} + MC_\delta (\Delta x)^2.$$

✓

**Corollary 9.** *To get convergence, the choice  $\delta = (\epsilon + \Delta x)^{1/3}$  shows that  $\|J_\delta f^\epsilon - f\|_{\infty, K} = O((\epsilon + \Delta t + \Delta x)^{1/3})$ , which implies formal convergence as  $\epsilon, \Delta t$ , and  $\Delta x \rightarrow 0$ .*

**Remark 10.** *The choice of  $\delta$  automatically defines the compact subset  $Q \subseteq I$  where we seek to reconstruct the unknown forcing term  $f$ .*

#### 4. Numerical trials

Let  $h = \Delta x = 1/M$  and  $k = \Delta t = 1/N$  be the parameters of the finite difference discretization of  $I$  with grid points  $(x_i, t_n) = (ih, nk)$ ,  $i = 0, 1, 2, \dots, M$ ,  $n = 0, 1, 2, \dots, N$  and set  $p = 3$  in the definition of the mollification kernel (2).

**4.1. Data generation.** In order to generate the necessary data to identify the source terms, we need first to solve the corresponding TFDE. To that end, we implement the unconditionally stable implicit finite difference method introduced in [22] utilizing Caputo's time partial fractional derivatives. We use the notation  $U(ih, nk)$  to indicate the computed approximation to the exact temperature distribution function  $u$  restricted to the grid point  $(ih, nk)$ .

The time marching scheme, for internal nodes, is given for  $n = 1$  by

$$\begin{aligned}\sigma_{\alpha,k}U(ih, 0) + f(ih, k) &= -\gamma a(ih, k)U((i-1)h, k) \\ &\quad + (\sigma_{\alpha,k} + 2\gamma a(ih, k))U(ih, k) \\ &\quad - \gamma a(ih, k)U((i+1)h, k), \quad i = 1, 2, \dots, M-1,\end{aligned}$$

and for  $n \geq 2$ ,

$$\begin{aligned}\sigma_{\alpha,k}U(ih, (n-1)k) - \sigma_{\alpha,k} \sum_{j=2}^n \omega_j^{(\alpha)} (U(ih, (n-j+1)k) - U(ih, (n-j)k)) \\ + f(ih, k) &= -\gamma a(ih, k)U((i-1)h, nk) + (\sigma_{\alpha,k} + 2\gamma a(ih, k))U(ih, nk) \\ &\quad - \gamma a(ih, k)U((i+1)h, nk) \quad (9) \\ i &= 1, 2, \dots, M-1, \quad n = 2, 3, \dots, N,\end{aligned}$$

with boundary conditions

$$U(0, nk) = u_0(0, nk), \quad U(1, nk) = u_1(1, nk), \quad n = 1, 2, \dots, N,$$

and initial temperature distribution

$$U(ih, 0) = u^0(ih, 0), \quad i = 0, 1, 2, \dots, M.$$

The parameters  $\gamma$ ,  $\sigma_{\alpha,k}$  and  $\omega_j^{(\alpha)}$  represent, respectively,

$$\gamma = \frac{1}{h^2}, \quad \sigma_{\alpha,k} = \frac{1}{\Gamma(1-\alpha)} \frac{1}{1-\alpha} \frac{1}{k^\alpha}$$

and

$$\omega_j^{(\alpha)} = j^{1-\alpha} - (j-1)^{1-\alpha}, \quad j = 1, 2, 3, \dots, N.$$

The numerical algorithm is consistent and the local truncation error is first order in time and second order in space.

Next, the discretized measured approximations of the temperature data functions are modeled by adding random errors to the computed data functions. That is,

$$u^\epsilon(ih, nk) = u_i^n + \epsilon_i^n, \quad i = 0, 1, \dots, M, \quad n = 0, 1, \dots, N,$$

where the  $(\epsilon_i^n)$ 's are Gaussian random variables with variance  $\sigma^2 = \epsilon^2$ .

**4.2. Numerical algorithm.** For computational efficiency, the original two-dimensional problem is reduced to a sequence of one-dimensional problems by first "marching", for example, in the  $t$  direction and then in the  $x$  direction.

The numerical algorithm is as follows:

- (1) At each fixed time level  $t_n$ , evaluate  $D_+ D_- (J_\delta u^\epsilon(x_i, t_n))$  from the noisy data  $u^\epsilon(x_i, t_n)$ ,  $i = 0, 1, 2, \dots, M$ , after automatically selecting the radius of mollification  $\delta_n = \delta_n(\epsilon)$  (see [24] for details).
- (2) Set  $\delta_x = \max\{\delta_0, \dots, \delta_N\}$ .

- (3) For each fixed space level  $x_i$ , evaluate  $\left(D_t^{(\alpha)} u^\epsilon(x_i, t_n)\right)_{\delta_i}$  from the noisy data  $u^\epsilon(x_i, t_n)$ ,  $n = 0, 1, 2, \dots, N$ , and automatically select the radius of mollification  $\delta_i = \delta_i(\epsilon)$ .
- (4) Set  $\delta_t = \max\{\delta_0, \dots, \delta_M\}$ .
- (5) Evaluate the source term  $J_\delta f^\epsilon(x_i, t_n)$  using equation (8) for  $(x_i, t_n) \in K \cap [3\delta_x, 1 - 3\delta_x] \times [3\delta_t, 1 - 3\delta_t]$ .

**Remark 11.** The algorithm uniquely defines the compact set  $Q = [3\delta_x, 1 - 3\delta_x] \times [3\delta_t, 1 - 3\delta_t]$  where the forcing term function  $f$  is approximately identified.

**4.3. Numerical examples.** In order to test the stability and accuracy of the method, we consider a selection of average noise perturbations  $\epsilon$ , and space and time discretization parameters,  $h$  and  $k$ . The errors at the “interior” discrete set  $K' = Q \cap K$  are measured by the weighted relative  $l_2$ -norm defined by

$$\frac{\left[ \frac{1}{\#K'} \sum_{(ih, nk) \in K'} |J_\delta f^\epsilon(ih, nk) - f(ih, nk)|^2 \right]^{\frac{1}{2}}}{\left[ \frac{1}{\#K'} \sum_{(ih, nk) \in K'} |f(ih, nk)|^2 \right]^{\frac{1}{2}}},$$

where  $\#K'$  indicates the number of grid points in  $K'$ .

The numerical examples presented next offer an interesting variety of possible behaviors for the source term  $f$ .

### Example 1.

Identify  $f(x, t) = 10e^{-\frac{1}{100}(x-0.5)^2} e^{-\frac{1}{100}(t-0.5)^2}$  if the temperature distribution satisfies the TFDE,  $0 < \alpha \leq 1$ ,

$$D_t^{(\alpha)} u(x, t) = \frac{\partial^2 u(x, t)}{\partial x^2} + f(x, t), \quad 0 < x < 1, \quad 0 < t < 1,$$

with boundary and initial conditions

$$\begin{aligned} u(0, t) &= 0, & 0 \leq t \leq 1, \\ u(1, t) &= 0, & 0 \leq t \leq 1, \\ u(x, 0) &= x(1-x), & 0 \leq x \leq 1. \end{aligned}$$

This prototype example emphasizes the estimation of a smooth impulse temperature at  $(x, t) = (0.5, 0.5)$ , from transient temperature data measured at the grid points of the unit square.

The TFDE is solved numerically for the time fractional orders  $\alpha = 0.10, 0.25, 0.50, 0.75$  and  $0.90$  using the implicit algorithm described previously with  $h = 1/100$  and  $k = 1/256$  to obtain the data temperature distribution for the source term identification problem.

After adding noise to the data at every point in  $K$ , for maximum noise levels  $\epsilon = 0.001, 0.01$  and  $0.05$ , the source term is reconstructed using formula (8) with

TABLE 1. Relative  $l_2$  errors as functions of  $\alpha$ .

Error norms at $x = 0.5$ , $\epsilon = 0.001$				
$\alpha$	$D_t^{(\alpha)}u$	$\frac{\partial^2 u}{\partial x^2}$	$f$	$f$ on $K'$
0.10	0.066	0.076	0.063	0.063
0.25	0.046	0.079	0.070	0.041
0.50	0.017	0.079	0.079	0.041
0.75	0.020	0.081	0.079	0.037
0.90	0.024	0.083	0.079	0.036

TABLE 2. Relative  $l_2$  errors as functions of  $\alpha$ .

Error norms at $x = 0.5$ , $\epsilon = 0.01$				
$\alpha$	$D_t^{(\alpha)}u$	$\frac{\partial^2 u}{\partial x^2}$	$f$	$f$ on $K'$
0.10	0.067	0.076	0.063	0.039
0.25	0.051	0.079	0.070	0.040
0.50	0.020	0.079	0.080	0.040
0.75	0.055	0.081	0.083	0.038
0.90	0.079	0.083	0.082	0.036

TABLE 3. Relative  $l_2$  errors as functions of  $\alpha$ .

Error norms at $x = 0.5$ , $\epsilon = 0.05$				
$\alpha$	$D_t^{(\alpha)}u$	$\frac{\partial^2 u}{\partial x^2}$	$f$	$f$ on $K'$
0.10	0.074	0.076	0.062	0.039
0.25	0.077	0.079	0.065	0.040
0.50	0.042	0.079	0.073	0.040
0.75	0.071	0.081	0.080	0.039
0.90	0.072	0.083	0.086	0.038

parameters  $h = 1/50, 1/100, 1/200$  and  $k = 1/128, 1/256$ . Tables 1-3 show the relative errors for  $D_t^{(\alpha)}u$ ,  $\frac{\partial^2 u}{\partial x^2}$  and  $f$  on the segment  $x = 0.5$  of  $K'$  and the relative error of the approximate values of  $f$  on the entire  $K'$  corresponding to the grid parameters  $h = 1/100$  and  $k = 1/256$ . These errors are typical since no significant changes occur if we consider values of the space and time discretization parameters in the tested intervals  $[1/50, 1/200] \times [1/128, 1/256]$ .

All the figures were prepared with  $h = 1/100$ ,  $k = 1/256$ ,  $\alpha = 0.75$  and  $\epsilon = 0.05$ . The exact data for the identification problem (solution of the direct

TFDE) as well as the noisy (perturbed) data are illustrated in Figures 1, 2 and 3. Figures 4 and 5 show the profile solutions of the TFDE at  $x = 0.5$  and  $t = 1.0$  for different values of the fractional order  $\alpha$ . It is possible to observe the rapid transients for small times and the larger asymptotic values of the temperatures for smaller values of  $\alpha$  justifying the “slow diffusion” characterization of the TFDE systems. It is also clearly visible the influence of the fractional order  $\alpha$  on the delay location of the maximum temperature peak.

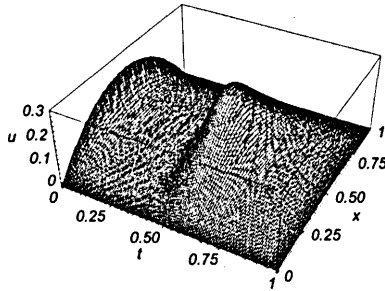


FIGURE 1. Exact Temperature,  $\alpha = 0.75$ .

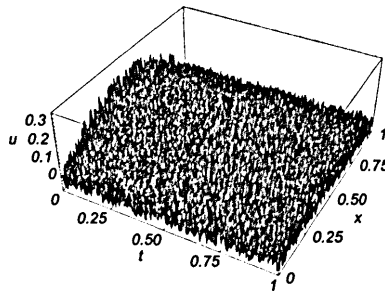


FIGURE 2. Noisy Temperature,  $\epsilon = 0.05$ .

Figure 6 depicts a profile of the reconstructed source term at the segment  $x = 0.5$  of  $K'$  together with the exact solution and, in Figures 7 and 8, we show the exact and reconstructed source terms on the entire domain  $K'$ .

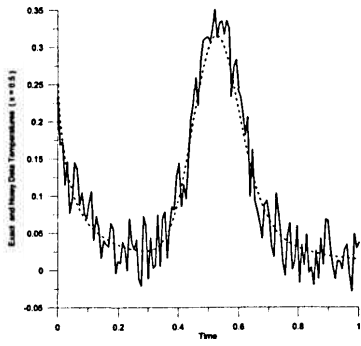


FIGURE 3.  $\alpha = 0.75, \epsilon = 0.05$ .

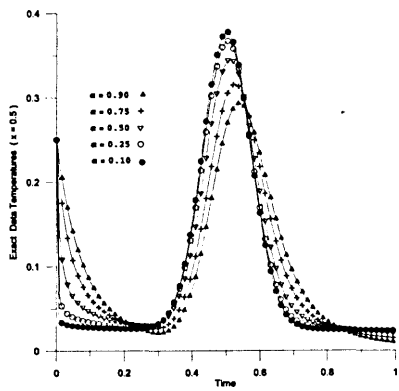


FIGURE 4. Exact Temperatures.

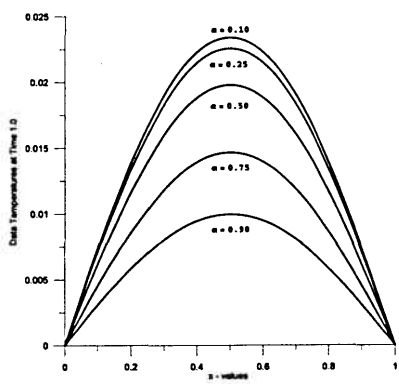


FIGURE 5. Exact Temperatures.

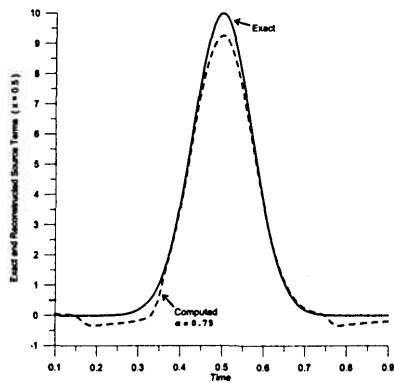


FIGURE 6.  $\alpha = 0.75, \epsilon = 0.05$ .

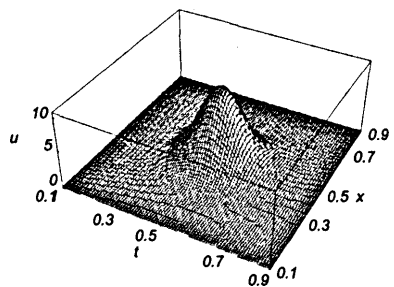


FIGURE 7. Exact Source Term.

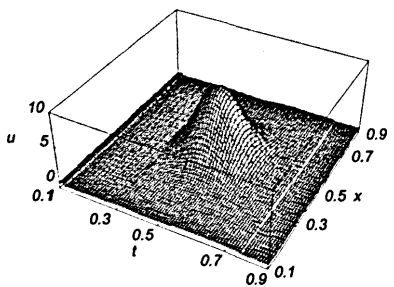


FIGURE 8. Computed Source Term.

**Example 2.**

Identify  $f(x, t) = (20 \cos(10x) + \sin(10x))e^{x-t}$  if the temperature distribution satisfies the TFDE,  $0 < \alpha \leq 1$ ,

$$D_t^{(\alpha)} u(x, t) = 1 + 0.005 x t \frac{\partial^2 u(x, t)}{\partial x^2} + f(x, t), \quad 0 < x < 1, \quad 0 < t < 1,$$

with boundary and initial conditions

$$\begin{aligned} u(0, t) &= 0, & 0 \leq t \leq 1, \\ u(1, t) &= 0, & 0 \leq t \leq 1, \\ u(x, 0) &= \sin(\pi x), & 0 \leq x \leq 1. \end{aligned}$$

This example exhibits a forcing term which is highly oscillatory in space. The TFDE is solved, and the source terms identified, with the same algorithms and parameters as in the first example.

Tables 4-6 show the relative errors for  $D_t^{(\alpha)} u$ ,  $\frac{\partial^2 u}{\partial x^2}$  and  $f$  on the segment  $x = 0.5$  of  $K'$  and the relative error of the approximate values of  $f$  on the entire  $K'$  corresponding to the grid parameters  $h = 1/100$  and  $k = 1/256$ . These errors are typical since no significant changes occur if we consider values of the space and time discretization parameters in the tested intervals  $[1/50, 1/200] \times [1/128, 1/256]$ .

TABLE 4. Relative  $l_2$  errors as functions of  $\alpha$ .

Error norms at $x = 0.5$ , $\epsilon = 0.001$				
$\alpha$	$D_t^{(\alpha)} u$	$\frac{\partial^2 u}{\partial x^2}$	$f$	$f$ on $K'$
0.10	0.103	0.037	0.043	0.032
0.25	0.094	0.037	0.046	0.031
0.50	0.092	0.037	0.057	0.026
0.75	0.075	0.050	0.081	0.035
0.90	0.091	0.052	0.081	0.032

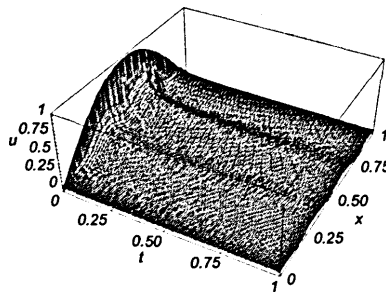
TABLE 5. Relative  $l_2$  errors as functions of  $\alpha$ .

Error norms at $x = 0.5, \epsilon = 0.01$				
$\alpha$	$D_t^{(\alpha)}u$	$\frac{\partial^2 u}{\partial x^2}$	$f$	$f$ on $K'$
0.10	0.102	0.038	0.043	0.031
0.25	0.093	0.037	0.046	0.030
0.50	0.093	0.037	0.056	0.036
0.75	0.076	0.049	0.081	0.035
0.90	0.092	0.052	0.081	0.037

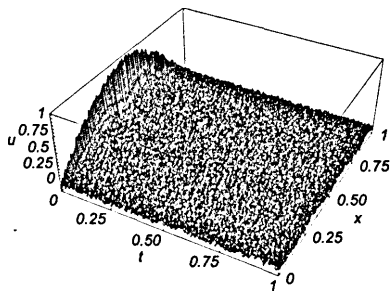
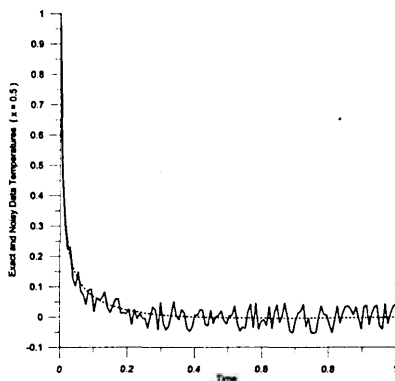
TABLE 6. Relative  $l_2$  errors as functions of  $\alpha$ .

Error norms at $x = 0.5, \epsilon = 0.05$				
$\alpha$	$D_t^{(\alpha)}u$	$\frac{\partial^2 u}{\partial x^2}$	$f$	$f$ on $K'$
0.10	0.103	0.037	0.043	0.032
0.25	0.094	0.037	0.046	0.030
0.50	0.093	0.037	0.056	0.026
0.75	0.081	0.050	0.080	0.035
0.90	0.095	0.051	0.082	0.037

All the figures were prepared with  $h = 1/100$ ,  $k = 1/256$ ,  $\alpha = 0.50$  and  $\epsilon = 0.05$ . The exact data for the identification problem (solution of the direct TFDE) as well as the noisy (perturbed) data are illustrated in Figures 9, 10 and 11.

FIGURE 9. Exact Temperature,  $\alpha = 0.5$ .

Figures 12 and 13 show the profile solutions of the TFDE at  $x = 0.5$  and  $t = 1.0$  for different values of the fractional order  $\alpha$ . It is again possible to

FIGURE 10. Noisy Temperature,  $\epsilon = 0.05$ .FIGURE 11.  $\alpha = 0.5$ ,  $\epsilon = 0.05$ .

observe the rapid transients for small times and the larger asymptotic values of the temperatures for smaller values of  $\alpha$ , typical of TFDE systems. Figure 14 depicts a profile of the reconstructed source term at the segment  $x = 0.5$  of  $K'$  together with the exact solution and, in Figures 15 and 16, we show the exact and reconstructed source terms on the entire domain  $K'$ .

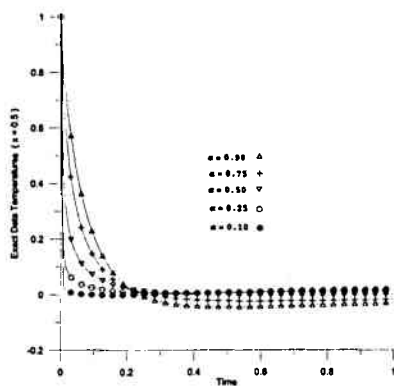


FIGURE 12. Exact Temperatures.

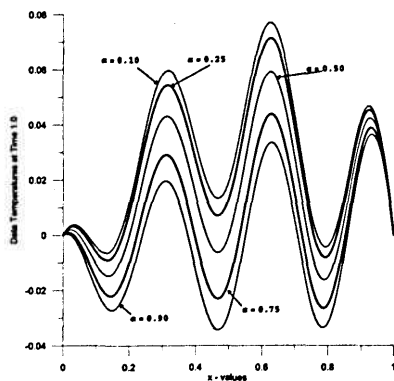
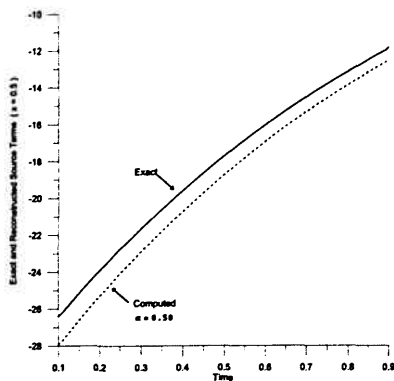


FIGURE 13. Exact Temperatures.

FIGURE 14.  $\alpha = 0.5$ ,  $\epsilon = 0.05$ .

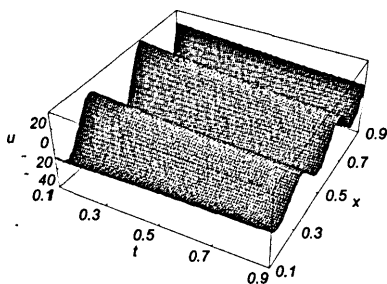


FIGURE 15. Exact Source Term.

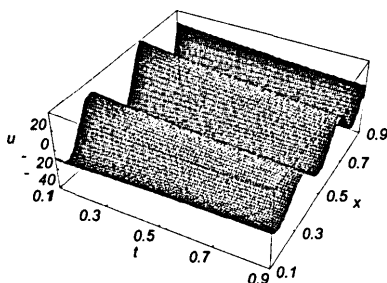


FIGURE 16. Computed Source Term.

Figures 1-16 give a clear qualitative indication of the approximate solutions obtained with the method. Further verifications of stability and accuracy are provided by the combination of parameters that yields the  $l_2$ -error norms data in Tables 1-6 for the source terms identification.

Inspection of Tables 1-6 indicates that in general, in both examples, errors increase slightly for increasing  $\alpha$  (more ill-posed problem) as more regularization is necessary to restore continuity with respect to perturbations in the data.

## References

- [1] ACOSTA, C., AND MEJÍA, C. Stabilization of explicit methods for convection diffusion equations by discrete mollification. *Computers Math. Applic.* 55 (2008), 368–380.
- [2] AGRAWAL, O. Solution for a fractional diffusion-wave equation defined in a bounded domain. *Nonlinear Dynamics* 29 (2002), 145–155.
- [3] CANNON, J., AND DUCHATEAU, P. Inverse problems for an unknown source in the heat equation. *Mathematical Analysis and Applications*, 75 (1980), 465–485.
- [4] CAPUTO, M. *Elasticà e Dissipazione*. Zanichelli, Bologna, 1969.

- [5] CHAVENT, G., AND JAFFRE, J. *Mathematical Models and Finite Elements for Reservoir Simulation*. North Holland, Amsterdam, 1986.
- [6] CHAVEZ, A. Fractional diffusion equation to describe Lévy flights. *Phys. Lett.* 239, A (1998), 13–16.
- [7] CHEN, C.-M., LIU, F., TURNER, I., AND ANH, V. A fourier method for the fractional diffusion equation describing sub-diffusion. *J. Comput. Phys.* (2007). doi: 10.1016/j.jcp.2007.05.012.
- [8] COLES, C., AND MURIO, D. A. Simultaneous space diffusivity and source term reconstruction in 2D IHCP. *Computers Math. Applic.* 42 (2001), 1549–1564.
- [9] DIETHELM, K., FORD, N., FREED, A., AND LUCHKO, Y. Algorithms for the fractional calculus: a selection of numerical methods. *Computer Methods in Applied Mechanics and Engineering* 194, g (2005), 743–773.
- [10] ELDEN, L. Solving an inverse heat conduction problem by a “method of lines”. *Journal of Heat Transfer* 119 (1997), 406–412.
- [11] EWING, R., AND LIN, T. *Parameter identification problems in single-phase and two-phase flow*. Birkhauser Verlag, Basel, 1989. International Series of Numerical Mathematics, 91.
- [12] EWING, R., LIN, T., AND FALK, R. *Inverse and Ill-Posed Problems*. Academic Press, Orlando, 1987, ch. Inverse and ill-posed problems in reservoir simulation, pp. 483–497. H. Engl and C. Groetsch eds.
- [13] LANGLANDS, T., AND HENRY, B. The accuracy and stability of an implicit solution method for the fractional diffusion equation. *Journal of Computational Physics* 205 (2005), 719–736.
- [14] LIU, F., ANH, V., AND TURNER, I. Numerical solution of the space fractional Fokker-Planck equation. *JCAM* 166 (2004), 209–219.
- [15] MAINARDI, F. *Fractals and Fractional Calculus Continuum Mechanics*. Springer Verlag, New York, 1997, ch. Calculus: some basic problems in continuum and statistical mechanics, pp. 291–348. A. Carpinteri and F. Mainardi eds.
- [16] MAINARDI, F., LUCHKO, Y., AND PAGNINI, G. The fundamental solution of the space-time fractional diffusion equation. *Fractional Calculus and Applied Analysis* 4 (2001), 153–192.
- [17] MEERSCHAERT, M., AND TADJERAN, C. Finite difference approximations for fractional advection-dispersion flow equations. *JCAM* 172 (2004), 65–77.
- [18] MEJÍA, C., AND MURIO, D. A. Numerical solution of the generalized IHCP by discrete mollification. *Computers Math. Applic.* 32, 2 (1996), 33–50.
- [19] MURIO, D. A. *The Mollification Method and the Numerical Solution of Ill-Posed Problems*. Wiley (Interscience), New York, 1993.
- [20] MURIO, D. A. *Inverse Engineering Handbook*. CRC Press, Boca Raton, Florida, 2002, ch. Mollification and Space Marching. K. Woodbury ed.
- [21] MURIO, D. A. On the stable numerical evaluation of Caputo fractional derivatives. *Computers and Mathematics with Applications* 51 (2006), 1539–1550.
- [22] MURIO, D. A. Implicit finite difference approximation for time fractional diffusion equations. Submitted, 2007.
- [23] MURIO, D. A. Stable numerical evaluation of Grünwald-Letnikov fractional derivatives. In *Proceedings of Inverse Problems, Design and Optimization Symposium* (Florida, 2007), G. S. D. et al., Ed., vol. I, Florida International University, pp. 44–48.
- [24] MURIO, D. A., MEJÍA, C., AND ZHAN, S. Discrete mollification and automatic numerical differentiation. *Computers Math. Applic.* 35, 5 (1998), 1–16.
- [25] NANDA, A., AND DAS, P. Determination of the source term in the heat conduction equation. *Inverse Problems* 12 (1996), 325–339.
- [26] OLDHAM, K., AND SPANIER, J. *The Fractional Calculus*. Academic Press, New York, 1974.

- [27] PODLUBNY, I. *Fractional Differential Equations*. Academic Press, New York, 1999.
- [28] SAMKO, S., KILBAS, A., AND MARICHEV, O. *Fractional Integrals and Derivatives*. Gordon and Breach Sciences Publishers, London, 1993.
- [29] SHEN, S., LIU, F., ANH, V., AND TURNER, I. Detailed analysis of an explicit conservative difference approximation for the time fractional diffusion equation. *J. Appl. Math. Computing* 22, 3 (2006), 1–19.
- [30] WHEELER, M., Ed. *Numerical Simulations in Oil Recovery*. Springer-Verlag, New York, 1988.
- [31] YI, S., AND MURIO, D. A. Source terms identification for the diffusion equation. In *Proceedings Fourth International Conference on Inverse Problems in Engineering* (Rio de Janeiro, 2002), H. Orlande, Ed., vol. I, pp. 100–107.
- [32] YUSTE, S., AND ACEDO, L. An explicit finite difference method and a new von Neumann-type stability analysis for fractional diffusion equations. *J. Numer. Anal. SIAM* 42, 5 (2005), 1862–1874.
- [33] ZHAN, S., AND MURIO, D. A. Surface fitting and numerical gradient computations by discrete mollification. *Computers and Mathematics with Applications* 37, 5 (1999), 85–102.
- [34] ZHUANG, P., AND LIU, F. Implicit difference approximation for the time fractional diffusion equation. *J. Appl. Math. Computing* 22, 3 (2006), 87–99.
- [35] ZHUANG, P., LIU, F., ANH, V., AND TURNER, I. New solution and analytical techniques of the implicit numerical methods for the anomalous sub-diffusion equation. *SIAM J. Numer. Anal.* to appear, 2007.

(Recibido en agosto de 2007. Aceptado en enero de 2008)

DEPARTMENT OF MATHEMATICAL SCIENCES  
 UNIVERSITY OF CINCINNATI  
 2600 CLIFTON AVE., CINCINNATI, OHIO 45221  
 CINCINNATI, OHIO, USA  
 e-mail: [diego@dmurio.csm.uc.edu](mailto:diego@dmurio.csm.uc.edu)

ESCUELA DE MATEMÁTICAS  
 UNIVERSIDAD NACIONAL DE COLOMBIA  
 CALLE 59A No. 63-20  
 MEDELLÍN, COLOMBIA  
 e-mail: [cemejia@unal.edu.co](mailto:cemejia@unal.edu.co)