

Applications of fractional calculus in solving Abel-type integral equations: Surface-volume reaction problem

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Abstract

In this paper we consider a class of partial differential equations that arise in modeling of surface-volume reactions. According to the literature, the class of differential equations we studied are normally solved using the Laplace transform method. In this study, we solve the equation using a fractional calculus approach. Several examples are considered to illustrate the method of solution. In this paper, for the first time, we encounter an order of the fractional derivative other than $\frac{1}{2}$ in an applied problem. This is the first in a series of papers which explore the applicability of fractional calculus in real-world applications, redefining the true nature of fractional calculus.

Keywords: Abel integral equation, Riemann–Liouville integral, Caputo fractional derivative, Fractional calculus, Surface-volume reactions

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1. Introduction

Until very recently, the fractional calculus had been a purely mathematical tool without apparent applications. Nowadays, fractional dynamical equations play a major role in the modeling of anomalous behavior and memory effects, which are common characteristics of natural phenomena [27, 46, 48]. The fact that fractional derivatives introduce a convolution integral with a power-law memory kernel makes the fractional differential equations an important model to describe memory effects in complex systems. Thus, it is seen that fractional derivatives or integrals appear naturally when modeling long-term behaviors, especially in the areas of viscoelastic materials and viscous fluid dynamics [41, 82].

Abel's study of the tautochrone problem [1] is considered to be the first application of fractional calculus to an engineering problem. In it one finds the path where the time it takes for an object to fall under the influence of gravity is independent of the initial position. The solution, which was solved using a fractional calculus approach, is now known to be a part of the inverted cycloid [1, 55].

Now it is not hard to find very interesting and novel applications of fractional differential equations in physics, chemistry, biology, engineering, finance and other areas of sciences that have been developed in the last few decades. Some of the applications include: diffusion processes [51, 76], mechanics of materials [14, 81], combinatorics [36, 77], calculus of variations [12, 13, 52, 60], signal processing [53], image processing

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[7], advection and dispersion of solutes in porous or fractured media [8], modeling of viscoelastic materials under external forces [20], bioengineering [49], relaxation and reaction kinetics of polymers [23], random walks [24], mathematical finance [75], modelling of combustion [42], control theory [64], heat propagation [67], modelling of viscoelastic materials [32] and even in areas such as psychology [4, 78]. The list is by no means complete. It is easy to find hundreds, if not thousands, of new applications in which the fractional calculus approach is more than welcome.

This is the first in a series of papers that seeks to find further potential applications of fractional calculus in solving real-world problems, a journey that can benefit both the understanding of profound complexities in the application, and the field of fractional calculus itself. As an application of the theory developed in this paper, we consider the surface-volume reaction problem. The governing equations of the mathematical formulation of such models naturally give rise to a nonlinear equation that contains a fractional integral embedded in it and have no solutions to date. A linear variation of this equation is normally solved using the Laplace transform method [16]. Thus, in this paper we extend the theory of fractional calculus methods by considering equations motivated by modeling the surface-volume reactions, and explore another interpretation of the fractional integral.

The remainder of this paper is organized as follows. The definitions and basic results are given in the second section. In Section 3, we give the main results, which are generalizations of Abel’s integral approach to the tautochrone problem. In section 4, we give illustrative examples to motivate our approaches. One of the main examples is the surface-volume reaction problem that have several very interesting applications in mathematical biology and engineering [17].

2. Basic Definitions and Preliminary Results

We adopt definitions given in [63] or in the encyclopaedic book by Samko *et al.* [74] here. We begin by introducing the concept of a *Riemann–Liouville fractional integral*:

Definition 2.1 ([63]). Let $\alpha > 0$ with $n - 1 < \alpha \leq n$, $n \in \mathbb{N}$, and $a < x < b$. The left- and right-Riemann–Liouville fractional integrals of order α of a function f are given by

$$J_{a+}^{\alpha} f(x) = \frac{1}{\Gamma(\alpha)} \int_a^x (x-t)^{\alpha-1} f(t) dt \quad \text{and} \quad J_{b-}^{\alpha} f(x) = \frac{1}{\Gamma(\alpha)} \int_x^b (t-x)^{\alpha-1} f(t) dt$$

respectively, where $\Gamma(\cdot)$ is Euler’s gamma function defined by

$$\Gamma(x) = \int_0^{\infty} t^{x-1} e^{-t} dt.$$

Non-local fractional derivatives are defined via fractional integrals [35, 74], while the local fractional derivatives are defined via a limit-based approach [38, 39]. A new class of controlled-derivative approach appeared in [5], though the results may not be considered as fractional derivatives according to the current literature [62]. In this work we utilize only the non-local Volterra-type definitions for the fractional derivative given below.

Definition 2.2 ([63]). The left- and right- *Riemann–Liouville fractional derivatives* of order $\alpha > 0$, $n - 1 < \alpha < n$, $n \in \mathbb{N}$, are defined by

$$\begin{aligned} D_{a+}^{\alpha} f(x) &= \frac{1}{\Gamma(n-\alpha)} \left(\frac{d}{dx} \right)^n \int_a^x (x-t)^{n-\alpha-1} f(t) dt, \\ D_{b-}^{\alpha} f(x) &= \frac{(-1)^n}{\Gamma(n-\alpha)} \left(\frac{d}{dx} \right)^n \int_x^b (t-x)^{n-\alpha-1} f(t) dt, \end{aligned}$$

respectively. It can be shown that in the case of $\alpha \in \mathbb{N}$ the above definitions coincide with the standard definition of the n^{th} -derivative of $f(x)$.

Definition 2.3 ([63]). The left- and right- *Caputo fractional derivatives* of order $\alpha > 0, n-1 < \alpha < n, n \in \mathbb{N}$, are defined by

$${}^C D_{a+}^\alpha f(x) = \frac{1}{\Gamma(n-\alpha)} \int_a^x (x-t)^{n-\alpha-1} f^{(n)}(t) dt \quad \text{and} \quad {}^C D_{b-}^\alpha f(x) = \frac{(-1)^n}{\Gamma(n-\alpha)} \int_x^b (t-x)^{n-\alpha-1} f^{(n)}(t) dt,$$

respectively. It can be shown that in the case of $\alpha \in \mathbb{N}$ the above definitions reduce to the standard definition of the n^{th} -derivative of $f(x)$. To see this, let us assume that $0 \leq n-1 < \alpha < n$, and $f(x) \in C^{n+1}[a, T]$. Then in the case of Caputo's derivative, we have, by integration by parts [63, p. 79],

$$\lim_{\alpha \rightarrow n} {}^C D_{a+}^\alpha f(x) = \lim_{\alpha \rightarrow n} \left(\frac{f^{(n)}(a)(x-a)^{n-\alpha}}{\Gamma(n-\alpha+1)} + \frac{1}{\Gamma(n-\alpha+1)} \int_a^x (x-\tau)^{n-\alpha} f^{(n+1)}(\tau) d\tau \right) \quad (1)$$

$$= f^{(n)}(a) + \int_a^x f^{(n+1)}(\tau) d\tau = f^{(n)}(x), \quad n = 1, 2, \dots \quad (2)$$

This shows that the Caputo derivative is a generalization of the integer-order derivative. A different proof of the fact in question, which does not use integration by parts, can be found on [15, pp. 49, 51] using an equivalent definition of the Caputo derivative. On the other hand, for the Riemann–Liouville derivative, the result follows easily since J_{a+}^0 is defined to be the identity operator and the fact that $D_{a+}^\alpha = D_{a+}^{[\alpha]} J_{a+}^{[\alpha]-\alpha}$ [15, p. 27].

The following relations between the Caputo and Riemann–Liouville fractional derivatives are noteworthy [15, 63]:

$${}^C D_{a+}^\alpha f(x) = D_{a+}^\alpha f(x) - \sum_{k=0}^{n-1} \frac{f^{(k)}(a)}{\Gamma(k-\alpha+1)} (x-a)^{k-\alpha} \quad (3)$$

and

$${}^C D_{b-}^\alpha f(x) = D_{b-}^\alpha f(x) - \sum_{k=0}^{n-1} \frac{f^{(k)}(b)}{\Gamma(k-\alpha+1)} (b-x)^{k-\alpha}. \quad (4)$$

The two relations in question have interesting properties. That is, if $f \in C^n[a, b]$ and $f^{(k)}(a) = 0, k = 0, 1, \dots, n-1$, then

$${}^C D_{a+}^\alpha f = D_{a+}^\alpha f,$$

and if $f^{(k)}(b) = 0, k = 0, 1, \dots, n-1$, then

$${}^C D_{b-}^\alpha f = D_{b-}^\alpha f.$$

The fractional integrals and derivatives also satisfy the following important properties: fractional operators are linear, that is, if L is a fractional integral or derivative, then

$$L(f+kg) = L(f) + kL(g)$$

for any functions $f, g \in C^n[a, b]$ or $f, g \in L^p(a, b)$ (as the case may be) and $k \in \mathbb{R}$. For any $\alpha, \beta > 0$, they also satisfy the following semigroup properties:

$$J^\alpha J^\beta = J^{\alpha+\beta} \quad \text{and} \quad D^\alpha D^\beta = D^{\alpha+\beta}.$$

Further, if $f \in L^\infty(a, b)$ or $f \in C^n[a, b]$ and $\alpha > 0$, then

$${}^C D_{a+}^\alpha J_{a+}^\alpha f = f \quad \text{and} \quad {}^C D_{b+}^\alpha J_{b+}^\alpha f = f. \quad (5)$$

Equation 5 will be the key property used to prove the main results of this paper. It also says that the Caputo derivative is the left-inverse of the Riemann–Liouville fractional integral. Unfortunately, the Caputo

derivative is not the right-inverse of the Riemann–Liouville integral. But, we have the following result concerning those two operators:

$$J_{a+}^{\alpha} {}^C D_{a+}^{\alpha} f(x) = f(x) - \sum_{k=0}^{n-1} \frac{f^{(k)}(a)}{k!} (x-a)^k,$$

and

$$J_{b-}^{\alpha} {}^C D_{b-}^{\alpha} f(x) = f(x) - \sum_{k=0}^{n-1} \frac{f^{(k)}(b)}{k!} (b-x)^k,$$

if $f \in C^n[a, b]$ and $\alpha > 0$.

The Caputo derivatives have some advantage over the Riemann–Liouville derivatives. One of the most important properties is that the Caputo derivative of a constant function is zero whereas the Riemann–Liouville derivative is not. From an analytical point of view, this result does not create difficulties though it is commonly not acceptable in the physical sense.

Using a convolution integral approach, Podlubny [65, 66] provided geometric and physical interpretations of fractional integration and fractional differentiation for the Riemann–Liouville fractional operators, Caputo derivatives, Riesz potentials and Feller potential. Several other attempts to provide geometric meanings to fractional operators can be found, for example, in the works by Ben Adda [2, 3]. Further approaches can be found in, for example, [25, 28, 29, 37, 47, 54, 57, 58, 69–71, 79, 83]. Among such approaches, as pointed out by Rutman [71], there were misunderstandings in some approaches which try to find interpretations of fractional integrals and derivatives [57]. Thus, one of the goals of this paper is to find concrete examples that can be directly related to the fractional operators so that we may find a better physical interpretation rather than building our own models. Further details of the approach can be found in Section 4 of this work.

The rest of the paper will adopt the following definitions of Volterra-type integrals.

Definition 2.4 ([31]). An integral equation of the form

$$w(t) = \int_a^t K(t, s)v(s) ds, \quad a \leq s \leq t \leq T, \tag{6}$$

is known as a *Volterra integral equation of the first kind* with kernel $K(t, s)$. Its kernel is said to be *non-singular* or *singular* depending on whether $K(t, s)$ is continuous or discontinuous on the triangular region $a \leq s \leq t \leq T$. In the special case where $K(t, s)$ has the form

$$K(t, s) = \frac{k(t, s)}{(t-s)^{\alpha}}, \quad 0 < \alpha < 1,$$

with $k(t, s)$ continuous on $a \leq s \leq t \leq T$, (6) is called a *generalized Abel integral equation* or an *integral equation of Abel type*.

For Abel type integral equations of the form

$$w(t) = \int_0^t \frac{k(t, s)}{(t-s)^{\alpha}} v(s) ds, \quad 0 \leq s \leq t \leq T, \quad 0 < \alpha < 1, \tag{7}$$

we have the following result [40, pp. 80–82]:

Theorem 2.5. *If*

- (i) $k(t, t) \neq 0, \quad 0 \leq t \leq T,$
- (ii) $k(t, s)$ has continuous partial derivatives up to order $m \in \{0, 1, 2, \dots\}$, and $\partial^{m+1}k(t, s)/\partial t^{m+1}$ is continuous on $0 \leq s \leq t \leq T,$
- (iii) $w(t) \in C^{m+1}[0, T]$ and $w^{(l)}(0) = 0, \quad (l = 0, 1, 2, \dots, m),$ and

(iv) $W(t) = \frac{d}{dt} \int_0^t \frac{w(s)}{(t-s)^{1-\alpha}} ds \in C[0, T],$

then $v(s) \in C^m[0, T]$ is unique.

It is interesting to see that condition (iv) of Theorem 2.5 is the Riemann–Liouville fractional derivative of order α for $0 < \alpha < 1$ though there is no explicit mention about such a derivative in the literature.

Now consider the following Abel integral equation of the first kind:

$$f(x) = \int_0^x \frac{g(t)}{(x-t)^\alpha} dt, \quad 0 < \alpha < 1, \quad 0 \leq x \leq b, \tag{8}$$

where $f \in C^1[a, b]$ is a given function satisfying $f(0) = 0$ and g is the unknown function to be determined. These Volterra-type integral equations are normally solved using the Laplace transform method [33, Chap. 8]. There are several other methods available in the literature for solving Abel’s integral equations of the first and second kind. Among them, the Chebyshev polynomial approach [6], orthogonal polynomial approach [56], Galerkin methods [19], collocation methods [11], Haar/CAS wavelet method [43, 72, 73] and Mikusinski’s operator approach [44] can be found in the references given.

Jahanshahi *et al.* [30] solved the problem given in (8) using a fractional calculus approach and arrived at the solution given below.

Theorem 2.6 ([30]). *The solution to (8) is*

$$g(x) = \frac{\sin(\pi\alpha)}{\pi} \int_0^x \frac{f'(t)}{(x-t)^{1-\alpha}} dt.$$

The interested reader may find a similar result in [44] and also in the work by Gelfand and Vilenkin [22, Section 5.5]. Those approaches are very similar to the method introduced by Abel in [1].

Continuing in the same direction, we shall solve a Volterra-type integral equation that involves two variable functions in the integrand, which contains partial derivatives. The method we describe here is new, to the authors’ knowledge.

Before elaborating on the new results, let us make some remarks about the notations that will be used in the rest of the paper.

2.1. Notations

Here we will go through some notation that is common to the current literature of the subject. It will be convenient to use operator notation. By J^α we will mean the fractional integral operator

$$J^\alpha f(x, t) = \frac{1}{\Gamma(\alpha)} \int_0^x \frac{f(\nu, t)}{(x-\nu)^{1-\alpha}} d\nu, \quad \alpha \in [0, 1].$$

Note this fractional integral is with respect to space. The reason for this will become clearer in section 5. If we take the fractional integral with respect to time, we will denote this by

$$J_t^\alpha f(x, t) = \frac{1}{\Gamma(\alpha)} \int_0^t \frac{f(x, \tau)}{(t-\tau)^{1-\alpha}} d\tau.$$

Also by $If(x, t)$, or simply by If , we will always mean an integral with respect to time:

$$If = \int_0^t f(x, \tau) d\tau.$$

Additionally we will use the notation

$$Igf = \int_0^t g(\tau) f(x, \tau) d\tau.$$

When dealing with fractional derivatives, we will always understand the fractional derivative in the Caputo sense

$$D^\alpha f = \frac{1}{\Gamma(1-\alpha)} \int_0^x \frac{1}{(x-\nu)^\alpha} \frac{\partial f(\nu, t)}{\partial \nu} d\nu.$$

We use a similar definition for the temporal fractional Caputo derivative

$$D_t^\alpha f = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{1}{(t-\tau)^\alpha} \frac{\partial f(x, \tau)}{\partial \tau} d\tau.$$

We are now ready to state our results.

3. Main Results

The following is the main result of this paper, which is motivated by a surface-volume reaction problem after taking into account transport effects. These equations are nonlinear in nature and have no exact solutions to date. Equations of this form can be found in the works of [16–18]. For example, the governing equations of this form can be found in Equations (2a) and (2b) of [18]. Further treatment of this class of equations can be found in Section 5.1 of this work.

Lemma 3.1. *Let C be a function such that its first partial derivative with respect to x exists. Let $0 < \alpha < 1$. Then the solution of the integral equation*

$$C(x, t) = \int_0^x \frac{\partial B}{\partial t}(x - \xi, t) \frac{d\xi}{\xi^\alpha}, \quad \text{with } B(x, 0) = 0, \tag{9}$$

is given by

$$B(x, t) = \frac{\sin(\pi\alpha)}{\pi} \int_0^t \int_0^x \frac{\partial C}{\partial x}(\xi, \tau) \frac{d\xi}{(x - \xi)^{1-\alpha}} d\tau. \tag{10}$$

Proof. We prove this first using a change of variable and then identifying (9) as a fractional integral of order α . To that end, let $x - \xi = \eta$ and $F(x; t) = \frac{\partial B}{\partial t}(x, t)$. Making this substitution, (9) becomes

$$C(x, t) = \int_0^x \frac{\partial B}{\partial t}(\eta, t) \frac{d\eta}{(x - \eta)^\alpha} d\eta. \tag{11}$$

This may be written as

$$C(x, t) = \Gamma(1 - \alpha) J^{1-\alpha} F(x; t). \tag{12}$$

Considering t to be a parameter and then taking the Caputo derivative of order $1 - \alpha$ of both sides of (12), we have

$$F(x; t) = \frac{1}{\Gamma(1 - \alpha)} D^{1-\alpha} C(x; t).$$

Upon integration and using the definition of the Caputo derivative we arrive at

$$\begin{aligned} B(x, t) &= \int_0^t F(x, \tau) d\tau \\ &= \frac{1}{\Gamma(1 - \alpha)\Gamma(\alpha)} \int_0^t \int_0^x \frac{\partial C}{\partial x}(\xi, \tau) \frac{d\xi}{(x - \xi)^{1-\alpha}} d\tau \\ &= \frac{\sin(\pi\alpha)}{\pi} \int_0^t \int_0^x \frac{\partial C}{\partial x}(\xi, \tau) \frac{d\xi}{(x - \xi)^{1-\alpha}} d\tau. \end{aligned} \tag{13}$$

This completes the proof. □

We also propose a new method for solving fractional-order integrodifferential equations. This method relies on transforming the integrodifferential equation into an integral equation, and then using Picard iterations to arrive at the solution. This approach is motivated by [45], where Loverro solves fractional integral equations by Picard iterations. Here we extend his approach to integrodifferential equations of fractional order.

Theorem 3.2. *Let \mathcal{L}_t be a second order linear partial differential operator of the form*

$$\mathcal{L}_t = \frac{\partial^2}{\partial t^2} + \phi(t) \frac{\partial}{\partial t} + \theta(t),$$

for some differentiable functions ϕ, θ . Let $y(t)$ be such that

$$\mathcal{L}_t y = 0, \tag{14}$$

with $y(t) \neq 0$ for all t . Then if $f(x, t)$ is continuous on $[0, 1] \times [0, T]$, the problem

$$\mathcal{L}_t B = J^\alpha \frac{\partial B}{\partial t} + f, \quad \text{with } B(x, 0) = \frac{\partial B}{\partial t}(x, 0) = 0 \tag{15}$$

on $[0, 1] \times [0, T]$ has a unique solution given by

$$B(x, t) = \sum_{n=0}^{\infty} y (K_2)^n (K_1 f), \tag{16}$$

where K_1, K_2 , and g are defined by

$$\begin{aligned} K_1(\rho) &:= I g(-\phi, -y) I g(\phi, y) y^{-1} J^\alpha \rho, \\ K_2(\rho) &:= I g(-y, -\phi) (J^\alpha g \rho - J^\alpha I \frac{\partial(gy^{-1})}{\partial t}(\rho)), \\ g(y, \phi) &:= \exp \left(I \left(2 \frac{dy}{dt} y^{-1} + \phi \right) \right). \end{aligned}$$

Proof. To prove existence we will transform equation (15) into a linear integral equation, and then use an inductive (iterative) process to arrive at the solution. In order to do this, an integrating factor method would be helpful. However, with the equation in its current form, we are unable to do so due to the presence of the term θB . To eliminate this we will proceed with an *ansatz* of the form

$$B(x, t) = b(x, t)y(t),$$

where y solves the homogenous equation (14) and $y(t) \neq 0$ for any $t \neq 0$. Substituting this into (15) we obtain

$$\left(y \frac{\partial^2 b}{\partial t^2} + 2 \frac{\partial b}{\partial t} \frac{dy}{dt} + b \frac{d^2 y}{dt^2} \right) + \phi \left(y \frac{\partial b}{\partial t} + b \frac{dy}{dt} \right) + \theta b y = J^\alpha \frac{\partial}{\partial t} (y b) + f.$$

However since y is a solution of $\mathcal{L}_t = 0$, we have

$$\frac{\partial^2 b}{\partial t^2} + \left(2 \frac{dy}{dt} y^{-1} + \phi \right) \frac{\partial b}{\partial t} = y^{-1} \left(J^\alpha \frac{\partial}{\partial t} (y b) + f \right).$$

This is a Bernoulli-type linear differential equation for the term $\frac{\partial b}{\partial t}$. Thus, following the standard procedure and multiplying by an integrating factor we have

$$\frac{\partial}{\partial t} \left(\exp \left(I \left(2 \frac{dy}{dt} y^{-1} + \phi \right) \right) \frac{\partial b}{\partial t} \right) = \exp \left(I \left(2 \frac{dy}{dt} y^{-1} + \phi \right) \right) y^{-1} \left(J^\alpha \frac{\partial}{\partial t} (y b) + f \right). \tag{17}$$

Before proceeding, for simplicity, let

$$g(y, \phi) := \exp \left(I \left(2 \frac{dy}{dt} y^{-1} + \phi \right) \right)$$

and

$$K_1(\rho) := Ig(-\phi, -y)Ig(\phi, y)y^{-1}\rho.$$

Then integrating (applying I to) each side of (17), multiplying each side by $g(-\phi, -y)$, and integrating again we arrive at

$$b = K_1 \left(J^\alpha \frac{\partial}{\partial t}(yb) + f \right).$$

In order to get the time derivative off of the term $\frac{\partial(yb)}{\partial t}$, we may apply integration by parts after applying Fubini's theorem. Indeed, since gy^{-1} is independent of the underlying space,

$$Igy^{-1}J^\alpha = IJ^\alpha gy^{-1}.$$

Therefore if $\frac{\partial B}{\partial t} = \frac{\partial(by)}{\partial t}$ is integrable (which we will show later),

$$\frac{1}{(x-\nu)^{1-\alpha}} \frac{\partial B}{\partial t}$$

is integrable on $[0, T] \times [0, 1]$. So we may apply Fubini's theorem

$$IJ^\alpha gy^{-1} \frac{\partial(yb)}{\partial t} = J^\alpha Igy^{-1} \frac{\partial(yb)}{\partial t},$$

and integration by parts to obtain

$$J^\alpha Igy^{-1} \frac{\partial(yb)}{\partial t} = J^\alpha gb - J^\alpha I \frac{\partial(gy^{-1})}{\partial t}(yb).$$

Now we define K_2b by

$$K_2b := Ig(-y, -\phi) \left(J^\alpha gb - J^\alpha I \frac{\partial(gy^{-1})}{\partial t}(yb) \right),$$

in order to cast our differential equation as an integral equation:

$$b = K_2b + K_1f. \tag{18}$$

Similarly we define the iterative sequence

$$b_{n+1} = K_2b_n + K_1f.$$

Then for some initial guess b_0 we have

$$b_{n+1} = \sum_{i=0}^n K_2^n K_1 f + K_2^{n+1} b_0. \tag{19}$$

If the sequence defined by (19) converges (see the Appendix), then we have

$$b = \sum_{i=0}^{\infty} K_2^n K_1 f, \tag{20}$$

which gives rise to (16) upon substitution of $B = yb$ into the product. Also observe that (18) implies uniqueness, for the associated homogenous problem is a linear integral equation for which 0 is a solution. \square

Remark 3.3. Clearly the assumption $B(x, 0) = 0$ is not necessary, and was just made to simplify the algebra. Certainly the theorem applies with more general initial conditions such as $B(x, 0) = h(x)$, $\frac{\partial B}{\partial t}(x, 0) = 0$; in those cases the form of (16) would simply change. Also note the second-order differential operator \mathcal{L}_t need not be constant coefficient. We require only the knowledge of a solution to the corresponding equation $\mathcal{L}_t y = 0$, with $y(t) \neq 0$. Solving (15) would be quite difficult using Laplace transform methods. Indeed, inverting the solution back from transform space would necessitate evaluating a very difficult contour integral.

We have proved the theorem when \mathcal{L}_t is a linear non-constant-coefficient, second-order differential operator. But similar results hold when \mathcal{L}_t is first order, or even when \mathcal{L}_t is a temporal Riemann–Liouville fractional derivative. Indeed, if we have

$$D_t^\beta B = J^\alpha B + f,$$

then

$$B = J_t^\beta J^\alpha B + J_t^\beta f,$$

which is a linear integral equation, and hence may be solved by Picard’s iteration method. The solution is given as

$$B = \sum_{n=0}^{\infty} (J_t^\beta J^\alpha)^n J_t^\beta f.$$

This may be summarized in the following theorem.

Theorem 3.4. *Let $B, f : [0, 1] \times [0, T] \rightarrow \mathbb{R}$ be differentiable with respect to t , and integrable with respect to x . Then the problem*

$$D_t^\beta B = J^\alpha B + f \quad B(x, 0) = f(x, 0) = 0 \tag{21}$$

has a unique solution given by

$$B = \sum_{n=0}^{\infty} (J_t^\beta J^\alpha)^n J_t^\beta f.$$

Proof. We first apply a fractional integral operator J_t^β to each side of (21). This transforms (21) into

$$B = J_t^\beta J^\alpha B + J_t^\beta f.$$

This is simply a linear integral equation, which may be solved using Picard’s iterations. Doing so, one obtains

$$B = \sum_{n=0}^{\infty} (J_t^\beta J^\alpha)^n (J_t^\beta f).$$

Convergence may be verified by an application of Weierstrass’s M -test. □

4. Illustrative Examples

Example 4.1. Consider the following Abel-type multivariate integral equation (of the first kind):

$$x^{4/3} = \int_0^x \frac{\partial B}{\partial t}(x - \xi, t) \frac{d\xi}{\xi^{2/3}} \quad \text{with } B(x, 0) = 0. \tag{22}$$

According to Lemma 3.1, taking $C(x, t) = x^{4/3}$, the solution of (22) is given by

$$\begin{aligned} B(x, t) &= \frac{\sin(\frac{2\pi}{3})}{\pi} \int_0^t \int_0^x \frac{\partial C}{\partial x}(\xi, \tau) \frac{d\xi}{(x - \xi)^{\frac{1}{3}}} d\tau \\ &= \frac{\sin(\frac{2\pi}{3})}{\pi} \int_0^t \int_0^x \frac{4}{3} \xi^{\frac{1}{3}} \frac{d\xi}{(x - \xi)^{\frac{1}{3}}} d\tau \\ &= \frac{4x}{3} \cdot \frac{\sin(\frac{2\pi}{3})}{\pi} \int_0^t \int_0^1 u^{\frac{1}{3}} (1 - u)^{-\frac{1}{3}} du d\tau, \quad \text{where } u = \frac{\xi}{x}, \\ &= \frac{4}{9} xt. \end{aligned} \tag{23}$$

Notice that we have used the properties of the $\Gamma(\cdot)$ function such as

$$B(\alpha, \beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha + \beta)} = \int_0^1 u^{\alpha-1}(1-u)^{\beta-1}du, \quad \Gamma(n+1) = n\Gamma(n), \quad \Gamma(\alpha)\Gamma(1-\alpha) = \frac{\pi}{\sin(\pi\alpha)}.$$

Next we will study some applications of our method that arise in modeling surface-volume reactions.

5. Applications

5.1. Setting

One of the major goals of this paper is to explore the applications of fractional calculus in solving real-world applications that arise in science, engineering and other disciplines. For example, stereology is concerned with the determination of three-dimensional objects from two- or one-dimensional data, and the extrapolation to three dimensions is based on the solution of a mathematical model derived using geometric probability and statistics. It is quite often the case that the model emerges in the form of an Abel integral equation [31, p. 123] given by

$$\int_a^\infty \left(\frac{x}{a}\right)^{\mu-1} \frac{g(\sqrt{x/a})}{(x-a)^\mu} dx = kz(a),$$

where $g(x)$ and $z(x)$ are probability density functions.

The Abel integral equations of the first/second kind with $\alpha = \frac{1}{2}$ also appear in a variety of problems in physics and chemistry; see, for example, the references in [10, 31, 61]. In this section we discuss a situation where, for the first time, we come across a fractional order different from $\frac{1}{2}$ in a real-world application.

The applications we consider here arise in the setting of *surface-volume reactions*. A surface-volume reaction is one where a buffer fluid containing ligand molecules is convected through a channel over a surface to which immobilized ligands (or receptors) are confined (see Figure 1). The scope of surface-volume reactions is very broad, and are of great importance in biology. Such reactions occur in blood clotting [26], drug absorption [9], and antigen-antibody interactions [68]. Surface-volume reactions also occur in DNA-protein interaction, which affects gene expression [16]. Additionally, purification processes often occur in channels with reactants embedded along the wall [16]. In order to experimentally study such reactions, scientists use an apparatus known as an *optical biosensor*. The use of optical biosensors is quite popular, with over 10,000 authors citing the use of an optical biosensors as of 2009 alone [80]. A schematic is depicted below.

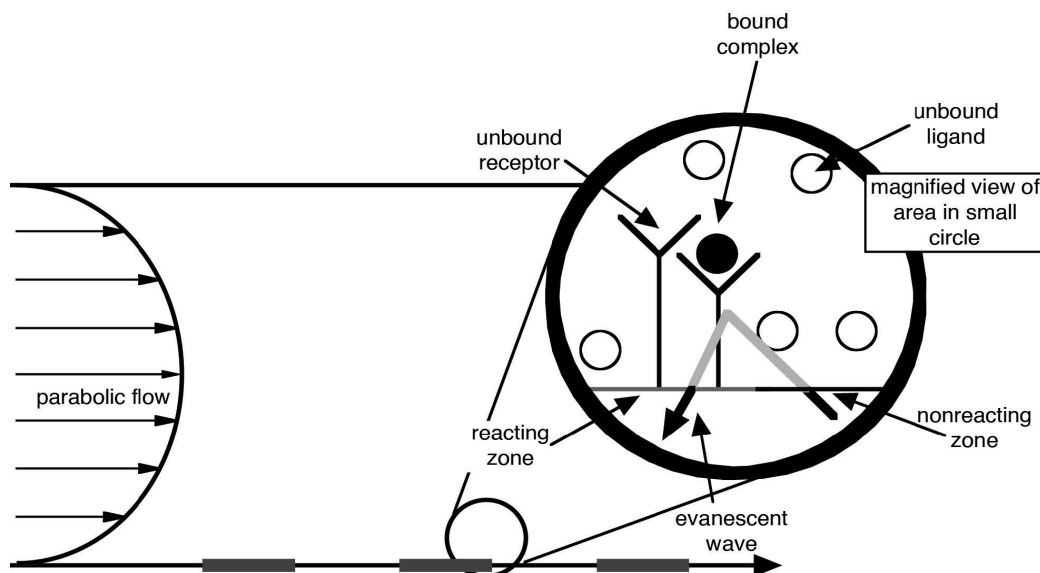
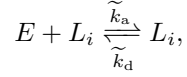


Figure 1: Cross-sectional schematic of the channel and binding/unbinding. Taken from [17].

In figure 1 one can see the unbound ligand being convected through the channel. As the unbound ligand molecules bind with the receptors on the surface, an evanescent wave is reflected off of the floor of the device. Refractive changes due to binding of the reactants are then averaged over the length of the ceiling to provide scientists with real-time mass measurements of the bound ligand concentration. The chemical kinetics at the boundary may be written as



where E represents an empty receptor and L_i denotes an unbound ligand molecule at the surface. A single ligand may bind with each receptor. The parameter \tilde{k}_a represents the dimensional reaction rate of ligand binding, and \tilde{k}_d represents the dimensional dissociation rate. Herein we will denote dimensional quantities with a tilde. Also we denote the dimensionless concentration of bound receptor sites at the surface by

$$[EL_i] = B, \quad [L_i] = C.$$

In general $C = C(x, y, t)$, and because there are only receptor sites on the floor of the channel, B is a function of x and t only. Following [16] we have scaled both the dimensional bound ligand concentration \tilde{B} and the dimensional unbound concentration \tilde{C} , so that the dimensionless variables B, C are between 0 and 1. Since there are no other sources or sinks, the bound ligand will change only due to association or dissociation:

$$\frac{\partial B}{\partial t} = (1 - B)C(x, 0, t) - KB, \quad B(x, 0) = 0. \quad (24)$$

Here K is a dimensionless parameter containing the ratio of the association and dissociation coefficients \tilde{k}_a, \tilde{k}_d . The term $(1 - B)C$ represents a bimolecular production term, and $-KB$ represents dissociation. If the unbound ligand concentration at the boundary $C(x, 0, t)$ were uniform, taking $C = 1$ gives the following solution of (24):

$$B(t) = \frac{1}{K + 1} \left[1 - e^{-t/(K+1)} \right].$$

There is initially no bound ligand in the channel, and as time progresses ligand molecules bind with the receptors until a balance between association and dissociation is reached, and the system reaches chemical equilibrium. Due to dissociation effects, this will happen before saturation.

In reality, transport will not be perfectly efficient. Edwards [16] has shown that $C(x, 0, t)$ takes the form of a fractional integral

$$C(x, 0, t) = 1 - \frac{\text{Da}}{3^{1/3}\Gamma(2/3)} \int_0^x \frac{\partial B}{\partial t} (x - \nu)^{-2/3} d\nu,$$

which may be expressed in terms of the Riemann-Liouville fractional integral

$$C(x, 0, t) = 1 - \frac{\text{Da}\Gamma(1/3)}{3^{1/3}\Gamma(2/3)} J^{1/3} \frac{\partial B}{\partial t}. \quad (25)$$

Substituting $C(x, 0, t)$ into the kinetics equation we arrive at

$$\frac{\partial B}{\partial t} = (1 - B) \left(1 - \frac{\text{Da}\Gamma(1/3)}{3^{1/3}\Gamma(2/3)} J^{1/3} \frac{\partial B}{\partial t} \right) - KB, \quad B(x, 0) = 0, \quad (26)$$

where Da denotes the Damköhler number, an important dimensionless parameter representing a ratio of reaction to diffusion. The Damköhler number

$$\text{Da} = \frac{\tilde{k}_a \tilde{L}^{1/3} \tilde{h}^{1/3} \tilde{R}_t}{\tilde{V}^{1/3} \tilde{D}^{2/3}}$$

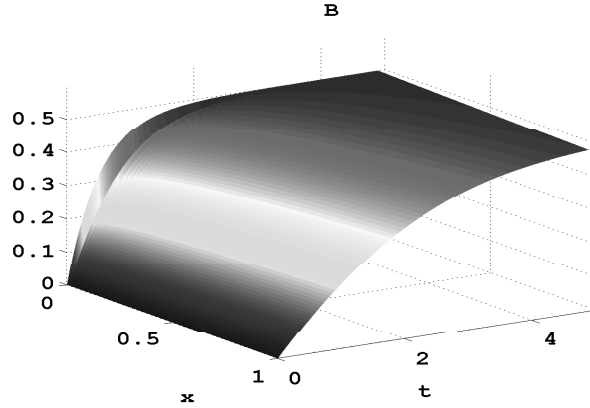


Figure 2: Numerical solution of (26), $Da = 2$, $K = 1$, computed numerically.

is a function of the dimensions of the channel \tilde{h}, \tilde{L} , characteristic velocity scale \tilde{V} , diffusion rate of the ligand molecules \tilde{D} , the reaction rate \tilde{k}_a , and the concentration of total receptor sites \tilde{R}_t . For physically realizable scenarios, Da is either $o(1)$ or $O(1)$ [16]. In Figure 2 we took $Da = 2$ to exaggerate transport effects; however in this paper we will only be consider the case where $Da = o(1)$. This corresponds to the parameter regime in which diffusion is much quicker than reaction. Therefore transport is quite efficient. Note that (24) is recovered in the limit as the Damköhler number goes to zero in (26). For a visualization of transport effects on the evolution of the bound ligand concentration, see Figure 2.

5.2. Physical Interpretation

We now discuss the physical interpretation of the fractional integral in (25). There are multiple time scales associated with the problem. There is a time scale for convection t_c , diffusion near the wall t_w , diffusion into the surface t_d , and reaction t . The flow *away from the wall* reaches equilibrium on the t_c time scale, and reaction occurs on the latter of the two time scales. The time scale for reaction is much slower than convection. Thus, one would expect that the unbound concentration at the boundary $C(x, 0, t)$ would be a perturbation away from the uniform outer concentration of 1:

$$C(x, 0, t) = 1 - Da c(x, t). \quad (27)$$

Edwards showed in ([16]) that

$$c(x, t) = \frac{\Gamma(1/3)}{3^{1/3}\Gamma(2/3)} J^{1/3} \frac{\partial B}{\partial t},$$

which gives (25) upon substitution into (27).

When transport effects are considered, initially there will be slightly more bound ligand upstream than downstream. This is due to the fact that the ligand will diffuse into the surface upstream first. Thus the fractional integral in (25) represents *upstream ligand depletion* [16]. If x is smaller, then less ligand will have already bound, thus (25) will be larger, and there will be more ligand available for binding at the surface upstream. Note that B is increasing so $\frac{\partial B}{\partial t}$ will be non-negative.

Thus far we have discussed only the *association phase* (or the *injection phase*) of the experiment. One can also model the *dissociation* or *wash phase* of the experiment. After studying the association phase of the experiment, scientists may wish to clean the optical biosensor for reuse. Therefore to clean the device scientists will simply convect only the buffer fluid through the channel. This has the effect of washing out all of the bound ligand. In the absence of transport this can be well modeled by the standard exponential decay curve

$$B(t) = \frac{e^{-t/(K+1)}}{1 + K}.$$

This is given as $C = 0$ in (24) with $B(0) = 1/(1 + K)$ (the equilibrium concentration in the association phase). However when considering transport effects, Edwards has shown in [17] that the kinetics process is governed by

$$\frac{\partial B}{\partial t} = (1 - B) \left[\frac{-\text{Da}}{3^{1/3!} (2/3)} \int_0^x \frac{\partial B}{\partial t} (x - \nu)^{-2/3} d\nu \right] - KB, \quad B(x, 0) = \frac{1}{1 + K},$$

or

$$\frac{\partial B}{\partial t} = (1 - B) \left(-\frac{\text{Da}! (1/3)}{3^{1/3!} (2/3)} J^{1/3} \frac{\partial B}{\partial t} \right) - KB. \quad (28)$$

Note that in this phase B is decreasing, so $\frac{\partial B}{\partial t}$ will be negative and the term

$$(1 - B) \left[\frac{-\text{Da}}{3^{1/3!} (2/3)} \int_0^x \frac{\partial B}{\partial t} (x - \nu)^{-2/3} d\nu \right]$$

will be positive. Observe that if $\text{Da} = 0$, transport is perfectly efficient and we recover the standard exponential decay model. The fractional integral in this phase has a slightly different interpretation. Ligand will bind in the wash phase only when ligand molecules dissociating upstream rebind with receptor sites downstream. If a receptor site is further downstream, then it is more likely that a ligand that has dissociated upstream will rebind with it. This is exactly what the fractional integral in (28) tells us. When x is very small, the fractional integral in (28) will also be small, and there will be a small possibility that a ligand molecule will rebind. Near the end of the channel, x will be close to 1, and inefficient transport will result in rebinding. Thus in this phase the fractional integral accounts for ligand rebinding due to inefficient transport. Notice that when Da is larger, the fractional integral will have a larger effect. This is because as the Damkohler number increases, reaction and diffusion (the transport mechanism) balance, and transport is less efficient. If transport is less efficient the nonuniformities will be greater, which is what (28) tells us.

5.3. Applications of Theorem 3.2

5.3.1. A Multiple Scale Expansion

One may propose a perturbation expansion to find approximate solutions of (26) where $\text{Da} = o(1)$ (the only parameter regime we are considering herein). A regular expansion of the form

$$B(x, t) = B_0(x, t) + \text{Da}B_1(x, t) + O(\text{Da}^2)$$

may be shown to be secular. However one may search for a multiple scale solution of the form:

$$B(x, t) = B_0(x, T, \tau) + \text{Da}B_1(x, T, \tau) + O(\text{Da}^2),$$

where

$$T = \text{Da}t \quad \text{and} \quad \tau = \left(1 + \sum_{n=2}^{\infty} \omega_n \text{Da}^n \right) t.$$

When doing so, in order to eliminate a secular term, one must solve the equation [16]

$$\frac{\partial f}{\partial t} = \frac{K}{3^{1/3!} (2/3)} \int_0^x f(\nu, t) (x - \nu)^{-2/3} d\nu, \quad f(x, 0) = -\frac{1}{\alpha}. \quad (29)$$

Edwards solved this equation by using a Laplace transform, solving the PDE in transform space, and mapping back *via* a term-by-term inversion of the Taylor series to the solution of the PDE in transform space.

We can also use fractional calculus methods to get this result. First let us rewrite (29) using the Riemann–Liouville integral:

$$\frac{\partial f}{\partial t} = r J^{1/3} f, \quad \text{where } r = \frac{! (1/3) K}{! (2/3) 3^{1/3}}.$$

Now integrating both sides gives

$$f + \alpha^{-1} = r \int_0^t J^{1/3} f dt.$$

Rearranging, we have

$$(1 - rIJ^{1/3})f = -\alpha^{-1}.$$

Inverting the operator on the left-hand side, we obtain

$$f = -\frac{1}{\alpha} \sum_{n=0}^{\infty} \frac{(rtx^{1/3})^n}{\Gamma(1 + n/3)n!}. \quad (30)$$

This is exactly the solution that Edwards arrives at in [16]. It is interesting to see that the expression in (30) is nothing but the Hadamard product of the two functions e^{rt} and the Mittag-Leffler function [63]

$$E_{\frac{1}{3}}(x^{1/3}) = \sum_{n=0}^{\infty} \frac{(x^{1/3})^n}{\Gamma(1 + n/3)}.$$

5.3.2. A Linearized Equation

A solution of (26) in closed form is very difficult to obtain. However, it may be of mathematical interest to consider a linear variant of (26) given by

$$\frac{\partial B}{\partial t} + \alpha B = 1 - \beta J^{1/3} \frac{\partial B}{\partial t}, \quad B(x, 0) = 0, \quad \beta = \frac{\text{Da}\Gamma(1/3)}{3^{1/3}\Gamma(2/3)}. \quad (31)$$

This equation is difficult to solve. Given the Abel-type integral operator one may try searching for solutions using Laplace transform methods. Indeed, via a Laplace transform, one arrives at a solution of the form

$$\widehat{B}(s, t) = \exp\left(\frac{t}{1 + \beta s^{1/3}}\right).$$

To the authors' knowledge there is no inverse transform to such function in the literature, and finding one would result in evaluating a difficult contour integral. One may then try inverting term-by-term.

$$\widehat{B} = \sum_{n=0}^{\infty} \left(\frac{t}{1 + \beta s^{1/3}}\right)^n (n!)^{-1}$$

which is again difficult to deal with. Thus we solve the linearized version by using a method similar to the one given in Theorem 3.2. First we multiply (31) by the integrating factor:

$$e^{\alpha t} \left(\frac{\partial B}{\partial t} + \alpha B\right) = e^{\alpha t} \left(1 - \beta J^{1/3} \frac{\partial B}{\partial t}\right),$$

which gives

$$B = \alpha^{-1}(1 - e^{-\alpha t}) - \beta IJ^{1/3} e^{\alpha(s-t)} \frac{\partial B}{\partial t},$$

where we have used the spatial independence of the exponential function. Next we interchange the order of integration by appealing to Fubini's Theorem:

$$B = \alpha^{-1}(1 - e^{-\alpha t}) - \beta J^{1/3} I e^{\alpha(s-t)} \frac{\partial B}{\partial t}.$$

Note an integration by parts gives

$$I \left(e^{\alpha(s-t)} \frac{\partial B}{\partial t} \right) = B - \alpha I e^{\alpha(s-t)} B.$$

This implies

$$B = \alpha^{-1}(1 - e^{-\alpha t}) - \beta J^{1/3}(B - \alpha I e^{\alpha(s-t)} B),$$

or rearranging,

$$[1 - \beta J^{1/3}(-1 + \alpha I e^{\alpha(s-t)})]B = \alpha^{-1}(1 - e^{-\alpha t}).$$

By inverting the operator on the left-hand side, after some algebra we arrive at

$$B = \sum_{n=0}^{\infty} \frac{(\beta x^{1/3})^n}{\Gamma(1 + n/3)} \left(\sum_{j=0}^n \binom{n}{j} (-1)^{n-j} \alpha^j (I e^{\alpha(s-t)})^j \alpha^{-1}(1 - e^{-\alpha s}) \right).$$

Here $(I e^{\alpha(s-t)})^j$ denotes an iterated j -fold integral

$$(I e^{\alpha(s-t)})^j \alpha^{-1}(1 - e^{-\alpha s}) = \underbrace{\int_0^t e^{\alpha(s-t)} \dots \int_0^t e^{\alpha(s-t)} \alpha^{-1}(1 - e^{-\alpha s}) ds \dots ds}_{j \text{ times}}$$

Convergence and differentiability follow from applications of the M -test.

6. Conclusion

Recently fractional calculus has been an area that is rich in application. We have found yet another application of fractional calculus in modeling surface-volume reactions. In particular, we have considered applications that occur when scientists simulate surface-volume reactions experimentally in an optical biosensor. We have seen that when modeling surface-volume reactions in optical biosensors, the fractional integral may be interpreted as a *ligand depletion term* during the injection phase of the experiment. In the dissociation phase the fractional integral represents ligand rebinding due to inefficient transport. Thus we have another interpretation to a centuries-old problem: “what is meant by a fractional integral operator?” This is also the first time we identify a fractional integral with order other than $\frac{1}{2}$ in an engineering problem.

Motivated by equation (26), we have considered several related equations. We have shown that these equations may be solved using fractional differentiation and integration. Additionally we have extended the approach in [45] to non-constant-coefficient partial integrodifferential equations. Attempting to solve the equations considered herein using Laplace transforms would be difficult to impossible. By considering equations motivated by the chemical kinetics in surface-volume reactions, we have been able to extend the theory of fractional calculus methods to more naturally occurring applications. It is of no doubt that further applications of the fractional derivative and integral are yet to be discovered. In the future we plan to use such applications to further enrich the theory and mathematical power of fractional calculus.

Appendix

It is left to show that (19) converges to (20), and that b is actually twice differentiable with respect to time. To prove this we show that each one of the series

$$\sum_{n=0}^{\infty} K_2^n(K_1)f \tag{32}$$

$$\sum_{n=0}^{\infty} \frac{\partial}{\partial t} K_2^n(K_1)f \tag{33}$$

$$\sum_{n=0}^{\infty} \frac{\partial^2}{\partial t^2} K_2^n(K_1)f \tag{34}$$

converge uniformly, and to do so we will apply the Weierstrass M -test.

To apply Weierstrass we will first need to show that the function $K_1f(x, t)$ is continuous in x and t . We will actually show that it is twice differentiable with respect to t . Now by definition

$$\begin{aligned} K_1(f(x, t)) &= Ig(-\phi, -y)Ig(\phi, y)y^{-1}f \\ &= \underbrace{\int_0^t g(-\phi, -y) \int_0^\tau \underbrace{g(\phi, y)y^{-1}f(x, s)}_1 ds}_{2} d\tau. \end{aligned}$$

Since f is continuous in x , so is K_1f . Also since f is a continuous function of t , $g(\phi, y)$ is a composition of differentiable functions, and y^{-1} is differentiable (this follows from the differentiability of y), then

$$\int_0^\tau g(\phi, y)y^{-1}f(x, s) ds$$

is a differentiable function of τ . For the same reasons the term labeled 2 is also the product of two differentiable functions with respect to time, thus

$$\int_0^t g(-\phi, -y) \int_0^\tau g(\phi, y)y^{-1}f(x, s) ds d\tau$$

is differentiable with respect to t . Therefore K_1f is twice differentiable with respect to time, and continuous with respect to space. Now since K_1f is a continuous function on a compact set, it is uniformly continuous and bounded. Thus there exists a constant C_1 such that for $(x, t) \in \mathcal{R} := [0, 1] \times [0, T]$, $|K_1f| \leq C_1$.

We are now in a position to apply the M -test; first we show uniform convergence of (32), and then move on to showing uniform convergence of (33) and (34). As a first step towards showing (32) converges uniformly, let

$$C_2 = \max_{\mathcal{R}} |g(-\phi, -y), g(\phi, y)| \quad \text{and} \quad C_3 = \max_{\mathcal{R}} \left| \frac{\partial(gy^{-1})}{\partial t} y^{-1} \right|,$$

and observe:

$$\begin{aligned} K_2|(K_1f)| &\leq K_2C_1 \\ &\leq (Ig(-\phi, -y)J^\alpha g(\phi, y) + Ig(\phi, -y)J^\alpha I \frac{\partial(ty^{-1})}{\partial t} y)C_1 \\ &= \frac{x^\alpha}{\Gamma(1+\alpha)} \left(tC_2^2 + \frac{C_2C_3t^2}{2} \right) C_1 \\ &\leq \frac{x^\alpha}{\Gamma(1+\alpha)} \left(TC_2^2 + \frac{C_2C_3T^2}{2} \right) C_1. \end{aligned}$$

Therefore inductively

$$\begin{aligned} K_2^n |K_1| &\leq \frac{x^{n\alpha}}{\Gamma(1+n\alpha)} \left(TC_2^2 + \frac{C_2 C_3 T^2}{2} \right)^n C_1 \\ &\leq \frac{1}{\Gamma(1+n\alpha)} \left(TC_2^2 + \frac{C_2 C_3 T^2}{2} \right)^n C_1 \end{aligned}$$

and since

$$\sum_{n=0}^{\infty} \frac{1}{\Gamma(1+n\alpha)} \left(TC_2^2 + \frac{C_2 C_3 T^2}{2} \right)^n C_1$$

is finite, our series converges uniformly. We now show (33) is convergent. The proof of this is quite similar. Letting

$$M_n = \frac{1}{\Gamma(1+n\alpha)} \left(TC_2^2 + \frac{C_2 C_3 T^2}{2} \right)^n,$$

one may show

$$\begin{aligned} \frac{\partial}{\partial t} K_2^n (K_1 f) &= \frac{\partial}{\partial t} K_2 (K_2^{n-1} (K_1 f)) \\ &\leq \frac{\partial}{\partial t} K_2 |K_2^{n-1} (K_1 f)| \\ &\leq \frac{\partial}{\partial t} K_2 M_{n-1} C_1 \\ &\leq \Lambda M_{n-1} C_1 \end{aligned}$$

Thus (33) is also bounded above by a convergent series, so (33) is convergent. An analagous argument may be given to show that the series (34) is convergent.

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