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FRACTIONAL CALCULUS

Models and Numerical Methods

Dumitru Baleanu
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Vol. 3 Fractional Calculus: Models and Numerical Methods
D. Baleanu, K. Diethelm, E. Scalas & J. J. Trujillo

Preface

Fractional Calculus deals with the study of so-called fractional order integral and derivative operators over real or complex domains and their applications. It has its roots in 1695, in a letter from de l'Hospital to Leibniz. Questions such as "What is understood by Fractional Derivative?" or "What does the derivative of order $1/3$ or $\sqrt{2}$ of a function mean?" motivated many brilliant scientists to focus their attention on this topic during the 18th and 19th centuries. For instance, we can mention Euler (1738, [211]), Laplace (1812, [329]), Fourier (1822, [226]), Abel (1823, [3]), Liouville (1832–1855, [347, 348]), Grünwald (1867, [252]), Letnikov (1868–1872, [337–339]), Riemann (1876, [478]), Laurent (1884, [333]), or Heaviside (1893–1912, [268, 269]).

It is well known that Abel implicitly applied fractional calculus in 1823 in connection with the tautochrone problem, which was modeled through a certain integral equation with a weak singularity of the type that appears in the so-called Riemann-Liouville fractional integral [4]. Therefore he can be considered the first scholar who investigated an interesting physical problem using techniques from what we today call fractional calculus. Later, Liouville tried to apply his definitions of fractional derivatives to different problems [347]. On the other hand, in 1882 Heaviside introduced a so-called operational calculus which reconciliated the fractional calculus with the explicit solution of some diffusion problems. Particularly, his techniques were applied to the theory of the transmission of electrical currents in cables [268]. For more historic facts about the development of the fractional calculus during these two centuries, the monographs by Oldham and Spanier [433], by Ross [490], by Miller and Ross [400] and Samko *et al.* [501] can be consulted.

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During the 20th century, up to 1985, we can list some of the pioneer researchers in this topic, such as Weyl (1917, [577]), Hardy (1917–1928, [259, 260]), Littlewood (1925–1928, [261, 262]), Levy (1937, [340]), Zygmud (1934–1945, [601, 602]), M. Riesz (1936–1949, [479, 480]), Doetsch (1937, [189]), Erdélyi (1939–1965, [207, 208]), Kober (1940, [320]), Widder (1941, [581]), Rabotnov (1948–1980, [453, 474]), Feller (1943–1971, [213, 214]), Maraval (1956–1971, [376, 377]), Sneddon (1957–1979, [526–528]), Gorenflo (since 1965, [245]), Caputo (since 1966, [131]), Dzherbashyan (1970, [197]), Samko (since 1967, [500]), Srivastava (since 1968, [530, 531]), Oldham (1969, [432]), Osler (1970, [436]), Caputo and Mainardi (since 1971, [136]), Love (since 1971, [351]), Oldham and Spanier (1974, [433]), Mathai and Saxena (since 1978, [383]), Ross (since 1974, [489]), McBride (since 1979, [385]), Nigmatullin (since 1979, [425]), Oustaloup (since 1981, [437, 438]), Bagley and Torvik (since 1983, [558, 558]), among others. As we will argue below, around 1985, new and fertile applications of fractional differential equations emerged and this field became part of applied sciences and engineering.

A fractional derivative is just an operator which generalizes the ordinary derivative, such that if the fractional derivative is represented by the operator symbol D^α then, when $\alpha = 1$, it coincides with the ordinary differential operator D. As a matter of fact, there are many different ways to set up a fractional derivative, and, nowadays, it is usual to see many different definitions. Here we must remark that, when we speak of fractional calculus, or fractional operators, we are not speaking of fractional powers of operators, except when we are working in very special functional spaces, such as the Lizorkin spaces.

Fractional differential equations, that is, those involving real or complex order derivatives, have assumed an important role in modeling the anomalous dynamics of many processes related to complex systems in the most diverse areas of science and engineering. However the interest in the specific topic of fractional calculus surged only at the end of the last century.

The theoretical interest in fractional differential equations as a mathematical challenge can be traced back to 1918, when O'Shaughnessy [435] gave an explicit solution to the differential equation $y^{(\alpha} = y/x$, after he himself had suggested the problem. In 1919, Post [457] proposed a com-

pletely different solution. Note that, at that time, this problem was not rigorously defined, since there was no mention of what fractional derivative was being used in the proposed differential equation. This explains why both authors found such different solutions, and why neither of them was wrong.

As one would expect, since a fractional derivative is a generalization of the ordinary derivative, it is going to lose many of its basic properties; for example, it loses its clear geometric or physical interpretation, the index law is only valid when working in specific functional spaces, the derivative of the product of two functions is difficult to compute, and the chain rule cannot be straightforwardly applied. It is natural to ask, then, what properties of fractional derivatives make them so suitable for modeling certain complex systems. We think the answer lies in the property exhibited by such systems of "non-local dynamics", that is, the processes' dynamics have a certain degree of memory and fractional operators are non-local, while the ordinary derivative is a local operator.

In 1974, after a joint research activity, Oldham and Spanier published the first monograph devoted to fractional operators and their applications in problems of mass and heat transfer [433]. In 1974, the First Conference on Fractional Calculus and its Applications took place at the University of New Haven, organized by B. Ross who edited the corresponding proceedings [489]. We can think of this year as the beginning of a new age for fractional calculus.

The stochastic interpretation for the fundamental solution of the ordinary diffusion equation in terms of Brownian motion has been known since the early years of 20th century. Physicists often mention Einstein as the pioneer in this field [200]. Indeed, Einstein's paper on Brownian motion had a large success and motivated further experimental work on the atomic and molecular hypothesis. However, five years before Einstein, L. Bachelier published his thesis on price fluctuations at the Paris stock exchange [46]. In this thesis, the connection was already made clear between Brownian motion and the diffusion equation. These results considered the position of a diffusing object as the sum of independent and identically distributed random variables leading to a Gaussian distribution in the asymptotic limit by virtue of the central limit theorem which was refined in the first half of the 20th century as well [215].

In 1949, Gnedenko and Kolmogorov [237] introduced a generalization of the classical central limit theorem for sums of random variables with infinite second moment converging to α-stable random variables. Almost simultaneously, Lévy and Feller also wrote seminal contributions leading to some controversy on priority [215]. In 1965, Montroll and Weiss [409] introduced a process in physics, later called continuous time random walk (CTRW) by Scher [408, 512, 513]. This process turned out to be very useful for the theoretical description of anomalous diffusion phenomena associated to certain materials [85]. CTRWs (also known as compound renewal processes in the mathematical community) are a generalization of the above mentioned method for normal diffusion processes. Therefore, they became the tool of choice for many applied scientists in order to characterize and describe anomalous diffusive processes from the mid-20th century until today.

The use of Laplace and Fourier integral transforms helps us in proving that, for a sub-diffusive process, the density function $u(x,t)$ of finding the diffusing particle in x at time t is the fundamental solution of the following time-fractional diffusion equation:

$$\Delta_x^2 u = k D_t^\beta u. \tag{1}$$

Such a connection lets us consider the CTRW models of the subdiffusive process as fractional differential models. Among the papers dealing with this fact there are Balakrishnan (1985, [51]), Wyss (1986, [586]), Schneider and Wyss (1989, [587]), Fujita (1990, [228–230]), Shlesinger, Zalavsky, and Klafter (1993, [521]), Metzler, Glöckle, and Nonnenmacher (1994, [394]), Zaslavsky (1994, [593]), Engheta (1996, [203]), Klafter, Shlesinger, and Zumofen (1996, [316]), Metzler and Nonnenmacher (1997, [397]), Metzler, Barkai, and Klafter (1999, [393]), Hilfer (2000, [280]), Anton (1995, [282]), and many more. For a comprehensive review, we recommend the excellent papers by Metzler and Klafter (2000–2004, [395, 396]). In these papers, the reader finds an accurate description of fractional diffusion models as well as a clear explanation of the role played by other linear or non-linear diffusive fractional models, such as the fractional Fokker-Planck equation.

The relationship between CTRWs and fractional diffusion will be dealt with in Chapters 6 and 7, as well as in several sections of Chapter 5. We must also point out that this is perhaps the first monograph presenting

modern numerical methods used to solve fractional differential equations (see Chapters 2 and 3).

As a result of many investigations in different areas of applied sciences and engineering and as a consequence of the relationship between CTRWs and diffusion-type pseudo-differential equations, new fractional differential models were used in a great number of different applied fields. We can mention material science, physics, astrophysics, optics, signal processing and control theory, chemistry, transport phenomena, geology, bioengineering and medicine, finance, wave and diffusion phenomena, dissemination of atmospheric pollutants, flux of contaminants transported by subterranean waters through different strata, chaos, and so on. Also, the reader can find many more references, e.g., in the monographs, [204, 280, 384, 442, 453, 550, 471, 108, 309, 365, 496, 517] and [66, 130, 145, 172, 370, 407, 508, 553, 543, 315, 92, 371]

The idea that physical phenomena, such as anomalous diffusive or wave processes, can be described with fractional differential models raises, at least, the following three fundamental questions:

- Are mathematical models with fractional space and/or time derivatives consistent with the fundamental laws and well known symmetries of the nature?
- How can the fractional order of differentiation be observed experimentally or how does a fractional derivative emerge from microscopic models?
- Once a fractional calculus model is available, how can a fractional order equation be solved (exactly or approximately)?

Of course, here, we must mention the very important contributions in nonlinear non-fractional differential models which were more studied by mathematicians than used by applied researchers, at least to describe the dynamics of processes within anomalous media, but this is beyond the scope of this book. However, we must remark the fractional differential models are a complementary tool to classical methods. The reader can consult the paper [105], where it is shown that strongly non-differentiable functions can be solutions of elementary fractional equations.

During the last 25 years there has been a spectacular increase in the use of fractional differential models to simulate the dynamics of many different anomalous processes, especially those involving ultra-slow diffusion. The

following table is only based on the Scopus database, but it reflects this state of affairs clearly:

Table 1. Evolution in the number of publications on fractional differential equations and their applications.

Words in title or abstract	1960–1980	1981–1990	1991–2000	2001–2010
Fractional Brownian Motion	2	38	532	1295
Anomalous Diffusion	185	261	626	1205
Anomalous Relaxation	21	23	70	61
Superdiffusion or Subdiffusion	0	22	121	521
Anomalous Dynamics Anomalous Processes Fractional Models Fractional Relaxation Fractional Kinetics Fractional Dynamics	11	24	128	443
Fractional Differential Equation Fractional Fokker-Planck Equation Fractional Diffusion Equation	1	1	74	943

On the other hand, and from a mathematical point of view, during the last five years we have been able to find many interesting publications connected with applications of classical fixed point theorems on abstract spaces to study the existence and uniqueness of solutions of many kinds of initial value problems and boundary value problems for fractional operators. See, e.g., [29, 327, 14, 424, 271, 13, 10, 547, 75, 177, 181].

For these reasons, we expect that fractional differential models will play an important role in the near future in the description of the dynamics of many complex systems. From our point of view, despite the attention given to it until the moment by many authors, only a few steps have been taken toward what may be called a clear and coherent theory of fractional differential equations that supports the widespread use of this tool in the applied sciences in a manner analogous to the classical case. Therefore we can find here a great number of both theoretical and applied open problems. For example, we think that three important kinds of such challenges, among others, are the following:

- In spite of the fact that there were several attempts to formulate a deterministic approach of fractional differential models in many different

areas of science and engineering, in general there have not been many rigorous justifications of such models. A deterministic approach to fractional differential models including a clear justification, as in the classical case, is an important open problem. Such an objective comes motivated mainly by the need to take into account the macroscopic behavior of anomalous processes not connected to stochastic theories. An example could be when studying the dynamics of ultrasonic waves through very irregular media, and there are many other potential examples. The first steps in this direction may have been done recently; see for example, [30, 486, 590, 589, 360, 485].

In addition, we recall the paper [428] where memory, expressed in terms of fractional operators, emerges from the initial model that does not "hint" to the presence of memory. Also, as an example, one can point to the literature on dielectric relaxation based on fractional kinetics [426] where differential equations containing non-integer operators describing the kinetic phenomena emerge from the self-similar structure of the medium considered. This approach recently received also its experimental confirmation [427].

- The introduction of a suitable fractional Laplacian for Dirichlet and Neumann problems associated to isotropic and anisotropic media. We must remark that, in the literature, at least three different approaches were used to solve such a problem in the isotropic case, namely the application of the well-known fractional power of operators, the hyper-singular inverse of one of the Riesz fractional integral operators of potential, and the characterization by means of the corresponding Fourier transform. The first two cases do not allow to work in wide functional spaces, whereas in the third one, the possibility exists not to determine with enough rigor the fractional Laplacian in the spatial field. We refer to [379, 499, 126, 125, 137, 127] for further details.
- The development of suitable and well-founded numerical methods to solve fractional ordinary and partial differential equations, so that applied researchers can refine their results, as in the classical case.

  We will devote two chapters of this book to this problem, where the reader can find a number of relevant references. In any case, this is still an important open field whose development will allow quicker advances in applied fields.

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Until now, our attention was focused on fractional differential equations and their applications. However, fractional operators had been mainly used for other objectives in the past. We will illustrate this fact with the following two examples connected with potential theory: the n-dimensional fractional operators introduced by Riesz (1932–1945), as a generalization of the Riemann-Liouville integral operators, were used to write the solution of certain ordinary partial differential equations explicitly [479]; Erdélyi and Sneddon (1960–1966) used the so-called Erdélyi-Kober fractional integral operators to solve explicitly certain dual integral equations (see [208, 527]).

Following such ideas, many other authors used fractional operators to generalize certain classical theories or to simplify classical problems. So, many special functions were expressed in terms of elementary functions by using fractional operators by Kiryakova [314]; the singularities of certain known ordinary differential equations were avoided in the framework of fractional calculus (see [487, 484]), or Riewe, Agrawal, Klimek, Baleanu *et al.* have initiated a fractional generalization of variational theory (see [481, 317, 15, 54, 62, 468, 34, 42, 298, 68, 542]), etc. Remarkable are the results obtained in control theory through the fractional generalization of the well-known PID controllers (see, for example, [442, 549, 550, 456, 441, 496, 407, 130]).

Therefore, we can use the label "fractional calculus models" when we refer to a generalization of a classical theory in the framework of fractional calculus. In this sense, in Chapter 4 and in a part of Chapter 5, we develop fractional generalizations of important classical theories. Below, we are going to explain such issues with more detail.

This book consists of a total of seven chapters, one appendix and an extensive bibliography.

Chapter 1 contains preliminary material that can be skipped by informed readers. This chapter is here to help the reader in reducing the use of external sources.

As we have seen, fractional-order models are a generalization of classical integer-order models. However, it turns out that these models are also in need of more general techniques in order to provide analytical solutions in closed form and/or qualitative studies of the solutions. As in the classical case, such techniques are not enough in many practical relevant cases. Thus

there is a substantial demand for efficient numerical techniques to handle fractional derivatives and integrals and equations involving such operators. Many algorithms were proposed for this purpose in the last few decades, but they tend to be scattered across a large number of different publications and, moreover, an appropriate and rigorous convergence analysis is often not available. Thus, a user who needs a numerical scheme for a particular problem often has difficulties in finding a suitable method. As a partial remedy to this state of affairs, in Chapters 2 and 3 we collect the most important numerical methods for practically relevant tasks. We have focused our attention on those algorithms whose behavior is well understood and that have proven to be reliable and efficient.

The fourth chapter is devoted to generalize the classical theory of Stirling numbers of first $s(n,k)$ and second kind $S(n,k)$ in the framework of the fractional calculus, basically using fractional differential and integral operators. Such special numbers play a very important role in connection with many applications, in particular in computing finite difference schemes and in numerical approximation methods. Such generalizations have been an open problem whose solution was approached by Butzer and collaborators, [111–115, 265], during the last years of the 20th century. We have worked out the mentioned generalization with respect to both parameters, n and k, so that they can be real or complex numbers, but keeping almost any known property corresponding to the classical numbers. Moreover, in this chapter, we introduce a number of important applications; for instance we connect the generalized Stirling functions with the corresponding infinity differences and with the fractional Hadamard derivative or with the fractional Liouville operators. On the other hand, we must remark that our treatment of this issue is not the ultimate one, even if we believe that our theory can open new and interesting perspectives to apply such results to approach to the calculus of infinite difference or fractional difference equations. The latter could be very important in the context of modeling the dynamics of anomalous processes.

Classical calculus of variations as a branch of mathematics is recognized for its fundamental contributions in various areas of physics and engineering. The history of variational calculus started already with problems well-known to Greek philosophers as well as scientists and contains illustrative contributions to the evolution of the science and engineering. During the last decade, when fractional calculus started to be applied intensively to

various problems related to real world applications, it was pointed out that it should be applied also to variational problems. As a result of this fusion the theory of fractional variational principles was created. This new theory consists of two parts, the first one is related to the mathematical generalization of the classical theory of calculus of variations and the second one involves the applications.

The fractional Euler-Lagrange equations recently studied are a new set of differential equations involving both the left and the right fractional derivatives.

As a result of interaction among fractional calculus, delay theory and time scales calculus, we observed that the new theory started to be generalized according to new results obtained in these fields. Also the applications of this new theory in so called fractional differential geometry started to be reported as well as with some promising generalizations of the classical formalisms in physics and in control theory.

An important feature of fractional variational principles is that they contain classical ones as a particular case when fractional operators converge to ordinary differential operators. Besides, fractional optimal control is largely developed and fractional numerical methods started to be applied to solve the fractional Euler-Lagrange equations. At this stage, we are confident that fractional variational principles will lead to new discoveries in several fields.

In Chapter 5, we introduce the reader of this book to the extension of variational calculus within the framework of fractional calculus, presenting a theory of fractional variational principles. Moreover, in the first part of the mentioned chapter, we consider the study of solutions for the corresponding fractional Euler-Lagrange equations, a new set of fractional differential equations involving both the left and right fractional derivatives.

In the second part of this chapter, we study the discrete and continuous case of the called fractional Hamiltonian dynamics, which generalizes the classical dynamics of Hamiltonian systems.

As already discussed, there is a deep connection between the fractional diffusion equation and the stochastic models for anomalous diffusion called CTRWs (continuous-time random walks). These processes, as discussed by physicists, are an instance of semi-Markov processes. This mild generaliza-

tion already leads to an infinite memory in time. Considered non-physical by several authors, spatial non-locality is connected to the power-law behavior of the distribution of jumps. All these phenomena are described by means of a suitable stochastic process, the fractional compound Poisson process with symmetric α-stable jumps which makes quite simple the proof of the generalized central limit theorem. This is the subject we study in Chapter 6.

In Chapter 7, we present an overview of the application of CTRWs to finance. In particular we give a brief presentation on the application of CTRWs, and implicitly fractional models, to option pricing and we point the reader to other applications such as insurance risk evaluation and economic growth models.

When tick-by-tick prices are considered, not only price jumps, but also inter-trade durations seem to vary at random. Therefore, as a first approximation, it is possible to describe durations as independent and identically distributed random variables. In this framework, position is replaced by log-price and jumps in position by tick-by-tick log-returns. The interesting case comes when inter-trade durations do not follow a exponential distribution.

The material covered in the seven chapters is complemented by an appendix where we explicitly provide the implementation of the algorithms described in the previous chapters, in several common programming languages.

Finally we include an extensive bibliography which, however, is far from being exhaustive.

During the time we have dedicated to write this monograph in this present form, the authors have gratefully received invaluable suggestions and comments from researches at many different academic institutions and research centers around the world. Special mention ought to be made of the help and assistance so generously and meticulously provided by colleagues Thabet Abdeljawad, Mohamed Herzallah, Fahd Jarad, Sami I. Muslih, Eqab M. Rabei, Margarita Rivero, Luis Rodríguez-Germá, and Luis Vázquez.

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