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This book mainly concerns the partial differential equations of fractional order and their numerical solutions. In Chapter 1, we briefly introduce the history of fractional order derivatives and the background of some fractional partial differential equations, in particular, their interplay with random walks. Chapter 2 is devoted to the definition of fractional derivatives and integrals from different points of view, from the Riemann-Liouville type, Caputo type derivatives and fractional Laplacian, to several useful tools in fractional calculus, including the pseudo-differential operators, fractional order Sobolev spaces, commutator estimates and so on. In chapter 3, we discuss some partial differential equations of wide interests, such as the fractional reaction-diffusion equation, fractional Ginzburg-Landau equation, fractional Landau-Lifshitz equations, fractional quasi-geostrophic equation, as well as some boundary value problems, especially the harmonic extension method. The local and global well-posedness, long time dynamics are also discussed. Last three chapters are devoted to the numerical aspects of fractional partial differential equations, mainly focusing on the finite difference method, series approximation method, Adomian decomposition method, variational iterative method, finite element method, spectral method and meshfree method and so on.

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Preface

In recent years, fractional-order partial differential equation models have been proposed and investigated in many research fields, such as fluid mechanics, mechanics of materials, biology, plasma physics, finance, chemistry and so on. Fractional-order differential equations, such as fractional Fokker-Plank equation, fractional nonlinear Schödinger equation, fractional Navier-Stokes equation, fractional quasi-geostrophic equation, fractional Ginzburg-Landau equation and fractional Landau-Lifshitz equation have clear physical backgrounds and opened up related new research fields. In fact, some mathematicians (such as L'Hôpital, Leibniz, Euler) began to consider how to define the fractional derivative as early as the end of the 17th century. In 1870s, Riemann and Liouville attained the definition of fractional derivative for a given function by extending the Cauchy integral formula,

$$ {}_0\mathrm{D}_t^{-v} f(t) = \frac{1}{\Gamma(v)} \int_0^t (t-\tau)^{v-1} f(\tau) \mathrm{d}\tau $$

where $\mathrm{Re}\, v > 0$. Nowadays, the commonly used fractional derivative definitions include Riemann-Liouville definition, Caputo definition, Grünwald-Letnikov definition and Weyl definition. Kohn and Nirenberg began the research on pseudo-differential operator in 1960s.

In recent years, we collected and summarized the researches on nonlinear fractional differential equations and their numerical methods for specific physical problems appearing in the fields of atmosphere-ocean dynamics and plasma physics, and studied the mathematical theories of these problems. This book introduces the latest research achievements in these areas, including some results of US, authors and our collaborators. To give a systematic understanding of fractional problems to our readers, we also introduce some basic concepts of the fractional calculus, their algorithms and basic properties, particularly, some numerical methods for fractional differential equations. The aim of this book is to show some recent developments in this research field for readers who are interested in this topic. Our expectation is that the readers, who want to engage in this field, can access to the frontier of this study after reading this book, and thus make certain progress.

Due to limited time and knowledge, errors and inadequacies are inevitable. Any suggestions and comments are welcome. Last but not least, we sincerely thank for the seminar members of Institute of Applied Physics and Computational Mathematics. We also thank Professor W. Chen and his team in Hohai University who translated the Chinese version into English of the first version, which reduced our burden of translation. We need to express our gratitude to all those unnamed as well.

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Contents

Chapter 1
Physics Background

Fractional differential equations have profound physical backgrounds and rich related theories, and are noticeable in recent years. They are equations containing fractional derivative or fractional integrals, which have applied in various disciplines such as physics, biology and chemistry. More specifically, they are widely used in dynamical systems with chaotic dynamical behavior, quasi-chaotic dynamical systems, dynamics of complex material or porous media and random walks with memory. The purpose of this chapter is to introduce the origin of the fractional derivative, and then some physical backgrounds of fractional differential equations. Due to space limitations, this chapter only gives some brief introductions. Even so, these are sufficient to show that the fractional differential equations, including fractional partial differential equations and fractional integral equations, are widely employed in various applied fields. However, further mathematical theories and numerical algorithms of fractional differential equations need to be studied. Interested readers can refer to more monographs and literatures.

1.1 Origin of the fractional derivative

The concepts of integer order derivative and integral are well known. The derivative $\mathrm{d}^n y/\mathrm{d}x^n$ describes the changes of variable y with respect to variable x, supported by profound physical backgrounds. Now the problem is how to generalize n into a fraction, even a complex number.

The long-standing problem can be traced back to the letter from L'Hôpital to Leibniz in 1695, in which it is asked like what the derivative $\mathrm{d}^n y/\mathrm{d}x^n$ is when $n = 1/2$. In the same year, the derivative of general order was mentioned in the letter from Leibniz to J. Bernoulli as well. The problem was also considered by Euler(1730), Lagrange(1849) *et al*, who gave some relevant insights. In 1812, by using the concept of integral, Laplace provided a definition of fractional derivative. When $y = x^m$, using the gamma function,

$$\frac{\mathrm{d}^n y}{\mathrm{d}x^n} = \frac{\Gamma(m+1)}{\Gamma(m-n+1)} x^{m-n}, \quad m \geqslant n, \tag{1.1.1}$$

was derived by Lacroix, who gives

$$\frac{\mathrm{d}^{1/2} y}{\mathrm{d}x^{1/2}} = \frac{2\sqrt{x}}{\sqrt{\pi}}, \tag{1.1.2}$$

when $y = x$ and $n = \frac{1}{2}$. This is consistent with the Riemann-Liouville fractional derivative in the present.

Soon later, Fourier (1822) gave the definition of fractional derivative through the Fourier transform. The function $f(x)$ can be expressed as a double integral

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(y) \cos \xi (x-y) \mathrm{d}\xi \mathrm{d}y,$$

and

$$\frac{\mathrm{d}^n}{\mathrm{d}x^n} \cos \xi (x-y) = \xi^n \cos \left(\xi (x-y) + \frac{1}{2} n\pi \right).$$

By replacing n with ν, and calculating the derivative under the integral sign, one can generalize the integer order derivative into the fractional order derivative

$$\frac{\mathrm{d}^\nu}{\mathrm{d}x^\nu} f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(y) \xi^\nu \cos \left(\xi (x-y) + \frac{1}{2} \nu\pi \right) \mathrm{d}\xi \mathrm{d}y.$$

Consider the Abel integral equation

$$k = \int_0^x (x-t)^{-1/2} f(t) \mathrm{d}t, \tag{1.1.3}$$

where f is to be determined. The right-hand side defines a definite integral of fractional integral with order 1/2. Abel wrote $\sqrt{\pi} \frac{\mathrm{d}^{-1/2}}{\mathrm{d}x^{-1/2}} f(x)$ for the right-hand component, then $\frac{\mathrm{d}^{1/2}}{\mathrm{d}x^{1/2}} k = \sqrt{\pi} f(x)$, which indicates that the fractional derivative of a constant is no longer zero.

In 1930s, Liouville, possibly inspired by Fourier and Abel, made a series of work in the field of fractional derivative, and successfully applied them into the potential theory. Since

$$D^m \mathrm{e}^{ax} = a^m \mathrm{e}^{ax},$$

the order of the derivative was generalized to be arbitrary by Liouville (ν can be a rational number, an irrational number, even a complex number)

$$D^{\nu}e^{ax} = a^{\nu}e^{ax}. \tag{1.1.4}$$

If a function f can be expanded into an infinite series

$$f(x) = \sum_{n=0}^{\infty} c_n e^{a_n x}, \qquad \mathrm{Re}\, a_n > 0, \tag{1.1.5}$$

its fractional derivative can be obtained as

$$D^{\nu}f(x) = \sum_{n=0}^{\infty} c_n a_n^{\nu} e^{a_n x}. \tag{1.1.6}$$

How can we obtain the fractional derivative if f cannot be written in the form of equation (1.1.5)? Liouville probably had noticed this problem, and he gave another expression by using the Gamma function. In order to make use of the basic assumptions (1.1.4), noting that

$$I = \int_0^{\infty} u^{a-1}e^{-xu}\mathrm{d}u = x^{-a}\Gamma(a),$$

one then obtains

$$\begin{aligned} D^{\nu}x^{-a} &= \frac{(-1)^{\nu}}{\Gamma(a)}\int_0^{\infty} u^{a+\nu-1}e^{-xu}\mathrm{d}u \\ &= \frac{(-1)^{\nu}\Gamma(a+\nu)}{\Gamma(a)}x^{-a-\nu}, \quad a > 0. \end{aligned} \tag{1.1.7}$$

So far, we have introduced two different definitions of fractional derivatives. One is the definition (1.1.1) with respect to $x^a (a > 0)$ given by Lacroix, the other is the definition (1.1.7) with regard to $x^{-a} (a > 0)$ given by Liouville. It can be seen that, Lacroix's definition shows that the fractional derivative of a constant x^0 is no longer zero. For instance, when $m = 0, n = \dfrac{1}{2}$,

$$\frac{\mathrm{d}^{1/2}}{\mathrm{d}x^{1/2}}x^0 = \frac{\Gamma(1)}{\Gamma(1/2)}x^{-1/2} = \frac{1}{\sqrt{\pi x}}. \tag{1.1.8}$$

However, in Liouville's definition, since $\Gamma(0) = \infty$, the fractional derivative of a constant is zero (despite Liouville's assumption $a > 0$). As far as which of the two definitions is the correct form of fractional derivative, Willian Center pointed out it can be attributed to how to determine $\mathrm{d}^{\nu}x^0/\mathrm{d}x^{\nu}$; and as De

Morgan indicated (1840), both of them may very possibly be parts of a more general system.

The present Riemann-Liouville's definition (R-L) of fractional derivative may be derived from N. Ya Sonin(1869) whose starting point was the Cauchy integration formula, from which the n^{th} derivative of f can be defined as

$$D^n f(z) = \frac{n!}{2\pi\mathrm{i}} \int_C \frac{f(\xi)}{(\xi - z)^{n+1}} \mathrm{d}\xi. \tag{1.1.9}$$

Using contour integration, the following generalization can be obtained (in which, Laurent's work were contributed!)

$${}_cD_x^{-\nu} f(x) = \frac{1}{\Gamma(\nu)} \int_c^x (x-t)^{\nu-1} f(t)\mathrm{d}t, \quad \mathrm{Re}\,\nu > 0, \tag{1.1.10}$$

where the constant $c = 0$ is commonly used. It is known as the Riemann-Liouville fractional derivative, i.e.,

$${}_0D_x^{-\nu} f(x) = \frac{1}{\Gamma(\nu)} \int_0^x (x-t)^{\nu-1} f(t)\mathrm{d}t, \quad \mathrm{Re}\,\nu > 0. \tag{1.1.11}$$

In order to make the integral convergent, a sufficient condition is $f(1/x) = O(x^{1-\varepsilon}), \varepsilon > 0$. An integrable function with this property is often referred to as belonging to the function of the Riemann class. When $c = -\infty$,

$${}_{-\infty}D_x^{-\nu} f(x) = \frac{1}{\Gamma(\nu)} \int_{-\infty}^x (x-t)^{\nu-1} f(t)\mathrm{d}t, \quad \mathrm{Re}\,\nu > 0. \tag{1.1.12}$$

In order to make the integral convergent, a sufficient condition is when $x \to \infty$, $f(-x) = O(x^{-\nu-\varepsilon})(\varepsilon > 0)$. An integrable function with this property is often referred to as belonging to the function of the Liouville class. This integral also satisfies the following exponential rule

$${}_cD_x^{-\mu}\,{}_cD_x^{-\nu} f(x) = {}_cD_x^{-\mu-\nu} f(x).$$

When $f(x) = x^a (a > -1)$, $\nu > 0$, from the equation (1.1.11), it is easy to get

$${}_0D_x^{-\nu} x^a = \frac{\Gamma(a+1)}{\Gamma(a+\nu+1)} x^{a+\nu}.$$

By using the chain law, it has $D[D^{-\nu} f(x)] = D^{1-\nu} f(x)$, then one can obtain

$${}_0D_x^{\nu} x^a = \frac{\Gamma(a+1)}{\Gamma(a-\nu+1)} x^{a-\nu}, \quad 0 < \nu < 1, \ a > -1.$$

Especially, when $f(x) = x$, $\nu = \frac{1}{2}$, Lacroix's equation (1.1.2) can be recovered; when $f(x) = x^0 = 1$, $\nu = \frac{1}{2}$, then the equation (1.1.8) can be recovered as well.

In addition, the Weyl's definition of fractional integral is frequently used now that

$$_xW_{\infty}^{-\nu}f(x)=\frac{1}{\Gamma(\nu)}\int_x^{\infty}(t-x)^{\nu-1}f(t)\mathrm{d}t,\qquad \mathrm{Re}\ \nu>0. \tag{1.1.13}$$

Using the R-L's definition of fractional derivative (1.1.12), and taking the transform $t=-\tau$, one obtains

$$_{-\infty}D_x^{-\nu}f(x)=-\frac{1}{\Gamma(\nu)}\int_{\infty}^{-x}(x+\tau)^{\nu-1}f(-\tau)\mathrm{d}\tau.$$

Then taking the transform $x=-\xi$, one derives the following equation

$$_{-\infty}D_{-\xi}^{-\nu}f(-\xi)=\frac{1}{\Gamma(\nu)}\int_{\xi}^{\infty}(\tau-\xi)^{\nu-1}f(-\tau)\mathrm{d}\tau.$$

Let $f(-\xi)=g(\xi)$, then the right end of Weyl's definition (1.1.13) can be recovered.

1.2 Anomalous diffusion and fractional advection-diffusion

Anomalous diffusion phenomena are ubiquitous in natural science and social science. In fact, many complex dynamical systems often contain anomalous diffusion. Fractional kinetic equations are usually an effective method to describe these complex systems, including diffusion type, diffusive convection type and Fokker-Planck type of fractional differential equations. Complex systems typically have the following characteristics. Firstly, the system typically contains a large diversity of elementary units. Secondly, strong interactions exist among these basic units. Thirdly, the anomalous evolution is non-predictable as time evolves. In general, the time evolution of, and within, such systems deviates from the corresponding standard laws. These systems are now applied in a large number of practical problems across disciplines such as physics, chemistry, engineering, geology, biology, economics, meteorology, and atmospheric. We will not give a systematic introduction of anomalous diffusion or fractional advection diffusion, but display some fractional differential equations for complex systems. We recommend the readers who are interested for more related monographs.

In the classical exponential Debye mode, the relaxation of the system usually satisfies the relation $\Phi(t)=\Phi_0\exp(-t/\tau)$. However, in complex systems, it often satisfies the exponential Kohlrausch-Williams-Watts relation $\Phi(t)=\Phi_0\exp(-(t/\tau)^{\alpha})$ for $0<\alpha<1$, or the asymptotic power law

$\Phi(t) = \Phi_0(1 + t/\tau)^{-n}$ for $n > 0$. In addition, the conversion from the exponential to power-law relationship can be observed in practical systems. Similarly, in many complex systems, the diffusion process no longer follows the Gauss statistics. Then, the Fick's second law is not sufficient to describe the certain transport behavior. In the classical Brownian motion, linear dependence of the time-mean-square displacement can be observed as

$$\langle x^2(t)\rangle \sim K_1 t. \tag{1.2.1}$$

However, in anomalous diffusion, the mean-square displacement is no longer a linear function of time. The power-law dependence is common, i.e., $\langle x^2(t)\rangle \sim K_\alpha t^\alpha$. Based on the index α of the anomalous diffusion, different anomalous diffusion types can be defined. When $\alpha = 1$, it is normal diffusion process. When $0 < \alpha < 1$, it is sub-diffusion process or dispersive, slow diffusion process with the anomalous diffusion index. When $\alpha > 1$, it is ultra-diffusion process or increased, fast diffusion process.

There have been extensive research results on anomalous diffusion process with or without an external force field situation, including:

(1) fractional Brownian motion, which can be traced back to Benoît Mandelbrot [153, 154];

(2) continuous-time random walk model;

(3) generalized diffusion equation [28];

(4) Langevin equation;

(5) generalized Langevin equation;

...

Among them, (2) and (5) appropriately describe the memory behavior of the system, and the specific form of the probability distribution function [162], however, it is insufficient to directly consider the role of the external force field, boundary value problem or the dynamics in the phase space.

1.2.1 The random walk and fractional equations

The following is a brief description of the random walk and the fractional diffusion equation. Considering the one-dimensional random walk, the test particle is assumed to jump randomly to one of its nearest neighbouring sites in discrete time interval Δt, with lattice constant Δx. Such a system can be described by the following equation

$$W_j(t + \Delta t) = \frac{1}{2}W_{j-1}(t) + \frac{1}{2}W_{j+1}(t),$$

where $W_j(t)$ represents the probability of the particle located at site j, at the time t, the coefficient $\frac{1}{2}$ means the walks of the particle are isotropic, i.e.

the probability of jumping to the left or right is $\frac{1}{2}$. Consider the continuum limit $\Delta t \to 0$, $\Delta x \to 0$, using the Talyor series expansion, we can get

$$W_j(t+\Delta t) = W_j(t) + \Delta t \frac{\partial W_j}{\partial t} + O((\Delta t)^2),$$

$$W_{j\pm 1}(t) = W(x,t) \pm \Delta x \frac{\partial W}{\partial x} + \frac{(\Delta x)^2}{2}\frac{\partial^2 W}{\partial x^2} + O((\Delta x)^3),$$

which leads to the diffusion equation

$$\frac{\partial W}{\partial t} = K_1 \frac{\partial^2}{\partial x^2} W(x,t), \qquad K_1 = \lim_{\Delta x \to 0, \Delta t \to 0} \frac{(\Delta x)^2}{2\Delta t} < \infty. \tag{1.2.2}$$

Based on simple knowledge of partial differential equations, the solution of the equation (1.2.2) can be expressed as

$$W(x,t) = \frac{1}{\sqrt{4\pi K_1 t}} \exp\left(-\frac{x^2}{4K_1 t}\right). \tag{1.2.3}$$

The function (1.2.3) is often called propagator, i.e. the solution of the equation (1.2.2) with initial data $W_0(x) = \delta(x)$. The solution of equation (1.2.2) satisfies the exponential decay law

$$W(k,t) = \exp(-K_1 k^2 t), \tag{1.2.4}$$

for individual mode in Fourier phase space.

For anomalous diffusion, we firstly consider the continuous-time random walk model. It is mainly based on the idea: for a given jump, the jump length and waiting time between two adjacent jumps are determined by a probability density function $\psi(x,t)$. The respective probability density functions of the jump length and waiting time are

$$\lambda(x) = \int_0^\infty \psi(x,t)\mathrm{d}t, \quad w(t) = \int_{-\infty}^\infty \psi(x,t)\mathrm{d}x. \tag{1.2.5}$$

Here $\lambda(x)\mathrm{d}x$ can be understood as the probability of the jump length in the interval $(x, x+\mathrm{d}x)$, and $w(t)\mathrm{d}t$ is the probability of a jump waiting time in time slice $(t, t+\mathrm{d}t)$. It is easy to see that if the jump time and jump length are independent, then $\psi(x,t) = w(t)\lambda(x)$. Different continuous-time random walk processes can be determined by the converging or diverging characteristics of the waiting time $T = \int_0^\infty w(t)t\mathrm{d}t$ accompanied with the variance of the jump length $\Sigma^2 = \int_{-\infty}^\infty \lambda(x)x^2\mathrm{d}x$. Now, the following equation can depict the continuous-time random walk model that

$$\eta(x,t) = \int_{-\infty}^\infty \mathrm{d}x' \int_0^\infty \mathrm{d}t' \eta(x',t')\psi(x-x',t-t') + \delta(x)\delta(t), \tag{1.2.6}$$

which links the probability density function $\eta(x,t)$ of the particle arrived at the site x at time t and the event of the particle arrived at the site x' at time t'. The second item on the right hand side represents the initial condition. Thus, the probability density function $W(x,t)$ of the particle at the site x at time t can be expressed as

$$W(x,t) = \int_0^t \mathrm{d}t' \eta(x,t')\Psi(t-t'), \quad \Psi(t) = 1 - \int_0^t \mathrm{d}t' w(t'). \tag{1.2.7}$$

The items of the equation (1.2.7) have the meanings: $\eta(x,t')$ means the probability density function of the particle at the site x at time t', and $\Psi(t-t')$ is the probability density function of the particle which does not leave until time t, thereby $W(x,t)$ is the the probability density function of the particle at the site x at time t. By using the Fourier transforms and Laplace transform, $W(x,t)$ satisfies the following algebraic relation [126]

$$W(k,u) = \frac{1-w(u)}{u} \frac{W_0(k)}{1-\psi(k,u)}, \tag{1.2.8}$$

where $W_0(k)$ represents the Fourier transform of the initial value $W_0(x)$.

When $w(t)$ and $\lambda(t)$ are independent, i.e. $\psi(x,t) = w(t)\lambda(x)$, and T and Σ^2 are finite, the continuous-time random walk model is asymptotically equivalent to the Brownian motion. Consider the probability density function of the Poisson waiting time $w(t) = \tau^{-1}\exp(-t/\tau)$, and $T = \tau$, and the Gauss probability density function of the jump length $\lambda(x) = (4\pi\sigma^2)^{-1/2}\exp(-x^2/(4\sigma^2))$, $\Sigma^2 = 2\sigma^2$. The Laplace transform and the Fourier transform have the following forms respectively, $w(u) \sim 1-u\tau+O(\tau^2)$ and $\lambda(k) \sim 1-\sigma^2k^2+O(k^4)$.

Consider a particular case: fractional time random walk, which leads to the fractional diffusion equation of describe the sub-diffusion process. In this model, the characteristic waiting time T is divergent and the variance Σ^2 of jump length is finite [196]. Then, we introduce the probability density function of the long-tail waiting time, whose asymptotic behavior and Laplace transform respectively satisfy, $w(t) \sim A_\alpha(\tau/t)^{1+\alpha}$ and $w(u) \sim 1-(u\tau)^\alpha$, but the specific form of $w(t)$ is insignificant. Taking the probability function $\lambda(x)$ of Gauss jumps into account, we can obtain the probability density function

$$W(k,u) = \frac{[W_0(k)/u]}{1+K_\alpha u^{-\alpha}k^2}. \tag{1.2.9}$$

Using the Laplace transform of the fractional integral [16, 69, 165, 175, 195]

$$\mathscr{L}\{{}_0D_t^{-p}W(x,t)\} = u^{-p}W(x,u), \quad p \geqslant 0,$$