Fractional Calculus for Hydrology, Soil Science and Geomechanics

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Foreword

This book offers a complete and self-contained overview of the theoretical aspects and applications of fractional calculus-based models in soil physics and hydrology, as well as poroelastic properties of porous media. It addresses water flow and solute movement in surface water, soils and groundwater systems. Further, this work also discusses some fractional generalizations of the main problems associated with flow and transport with these theories.

With the comprehensive and clear evidence of the practical implications of fractional calculus and the advantages of this theory to the current lore, this book represents a remarkable piece of literature that will certainly be a fundamental reference for those who wish to pursue theoretical studies and applications of fractional calculus in hydrology, soil science and related topics.

May 2019

Francesco Mainardi
University of Bologna
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Preface

This book focuses on the development of fractional calculus-based mathematical models and their applications in hydrology, soil science and mechanics of flow in porous media.

Fractional calculus has been widely applied to numerous fields since its inception in 1695. Hydrology, soil science, mechanics of flow in porous media and other branches of geoscience and environmental science are among the fields where different mathematical models based on fractional calculus are extensively used. In spite of the wide range of applications of fractional calculus, there is no single treatise which presents, in a systematic form, its background, theory, models and applications with examples in hydrology, soil science, mechanics of flow in porous media, and other related topics in geoscience. The reality at the moment is that extensive reports on the development of fractional calculus and its applications in the form of fractional partial differential equations (fPDEs) and fractional integral equations (fIEs) in these fields appear in a wide range of journals and some are scattered in a limited number of books.

In this book, I endeavor to bring together the essential mathematics of fractional calculus, particularly the theory of fPDEs and their applications as models and in related topics, for readers in hydrology, soil science, mechanics of flow in porous media and some related branches of geo-environmental sciences.

Furthermore, I present the majority of these mathematical models as fPDEs in different forms and, in limited cases, fIEs and fractional differential equations (fDEs) reported by others (in literature) and developed by myself (including some unpublished results). I have also cited more than 900 references through the length of the book, listed in the Bibliography, which include both important historical and contemporary contributions in fractional calculus and pertinent topics. I believe that these references are very valuable and can provide useful information to the readers.

I aim to present these materials as a summary of the most relevant reported models, along with my own research findings in these fields. With this objective, I hope the content of this book to be of interest to senior undergraduates and postgraduates for their studies, and useful for scientists, engineers and practitioners with an interest in the background, theory and applications of fractional calculus-based models in related fields.

I first became acquainted with the term Fractional Calculus in my initial days serving as a Senior Research Associate at the School of Mathematical Sciences, Queensland University of Technology (QUT) in Brisbane, Australia. At a School seminar in late 2000, I was sitting next to Professor Fawang Liu, a colleague at the School. In 2012, he was awarded the Mittag-Leffler prize at the *International Conference on Fractional Differentiation and Its Applications* (FDA'12) held in Nanjing, China, for his pioneer contributions to numerical methods for fPDEs and related models. I noticed that he was holding a book titled Fractional Differential Equations by Igor Podlubny. I asked, "Can differential equations be fractional?" From this point, I started learning fractional calculus, particularly, fPDEs and fDEs and their applications.

Having published some papers on fPDEs developed for analyzing water movement in soils and aquifers, since 2009, I have increasingly realized the absence of a compact book which systematically presents the fundamentals and the most relevant materials on fPDEs and their applications in hydrology, soil science and mechanics of flow in porous media. In April 2016, Mr. Raju Primlani at Science Publishers, CRC Press/Taylor & Francis Group contacted me for writing a book on certain issues, but I had not decided what to write then. I am thankful for Mr. Primlani for his communication over the past few years which eventually resulted in this book.

In October 2016, following my visit to Ningxia University, I met my uncle, Mr. Su Haidong, a retired public servant from the county of Longde, Ningxia, and an amateur poet and calligrapher. During one of our conversations, he suggested me to write a book on the topics I am working on. I promised him, and decided then, to write something on fPDEs and their applications. I am very grateful for his interest in my study and career as he has always been encouraging since my childhood.

I am extremely grateful to Professor Francesco Mainardi at the University of Bologna, Italy, who was awarded the Mittag-Leffler prize at the FDA'14 held in Catania, Italy, for his pioneer contributions to the applications of the Mittag-Leffler function in problems of fractional calculus. I communicated with him over six years ago regarding his papers as a part of the materials for my self-education on fPDEs and related topics. In December 2018, I also requested him to comment on the draft book chapters. With the help of Professor Mainardi, who also sent me some of the papers he had published, I was able to apply the continuous-time random walk (CTRW) theory to derive fPDEs and carry out related asymptotic analyses of the solutions of fPDEs, which resulted in my development of the models for water movement in soils (2014) and in aquifers (2015, 2017), all of which have been published in the Journal of Hydrology. Through my communication with Professor Mainardi, following his comment on my draft chapters in April 2019, I was informed of some 'fake' fractional derivatives, in his own words, in literature which are spurious definitions of fractional derivatives proposed by some authors in contrast to the classical definitions identified by Tarasov (doi.org/10.1016/j.cnsns.2018.02.019).

I am also very grateful to late Professor Rudolf Gorenflo, who was originally with the Free University of Berlin, Germany. I contacted him for some papers, particularly on fIEs, that were published by him and/or his colleagues and introduced me to the solutions of fIEs. Originally, I wrote to him in December 2018 to request for his comment on the book's manuscript, in addition to the comments of Professor Mainardi. However, I was sadly informed by his son Harry that Professor R. Gorenflo had passed away in October 2017.

The library staff at James Cook University have been extremely efficient and helpful by locating some very valuable and rare references which could be used and included for my writing. Following the submission of the manuscript of this book, the editorial staff at the CRC Press/Taylor & Francis Group have efficiently provided professional comments and suggestions before the manuscript went into production.

I thank my partner, Rosalind Gilroy, who has always been supportive, positive and interested in what I have been doing. She proofread the whole draft book for errors and suggested changes. Despite her training in economics and marketing, she was remarkable in identifying some typing errors of highly mathematical nature, such as the wrong limits in the definitions of left-hand and right-hand fractional derivatives and special functions, which could ideally be identified only by mathematicians.

I can say that this book is a result of teamwork which originated from an invitation from a publisher, the encouragement from my uncle for its inception, and references and comments from Professor Mainardi and Professor Gorenflo. The corrections and proofreading from Rosalind and the editors are essential for the present form of this book. My connection and cooperation with Professor Fawang Liu at QUT, since 1997, while I was working in New Zealand, has been crucial for me to realign my research directions in hydrological and environmental modelling closer with those of mathematicians. Without this teamwork, the publication of this book would be impossible. I thank you all! However, as the author, I am responsible for everything presented herein.

November 2019

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Chapter 1

Application of Fractional Calculus in Water Flow and Related Processes

1. Overview

Water and its movement on land, in soils and aquifers, and in the oceans support terrestrial and marine life on the Earth. Since the very ancient times, human settlements had to either be in the vicinity of viable water sources or build water storage facilities for their survival. In the first instance, the appearance of fresh water sources, in the form of rivers or springs, was essential for humans' survival and, notably, all the earliest civilizations were facilitated by the availability of fresh water such as along the river systems of Nile in Egypt, Tigris and Euphrates in Mesopotamia, Indus in India, and Huanghe (or Dahe, the Yellow River) in China. In the second situation wherein humans lived in dry areas or needed water for special purposes, water engineering works can be traced back to 3,200 BC (Biswas 1967) across the ancient civilizations.

In addition to meeting human survival and basic needs as an essential resource and commodity, water has been the object of spiritual, mythical, mythological, religious and philosophical activities. The earliest Greek philosopher Thales (624 BC–548 BC) (Cartledge 1998) is credited with the hypothesis that water was the underlying factor behind the development of the world. The great Chinese philosopher Laozi (or Laotzu) (~ 571 BC–~ 471 BC) reiterated the virtue of water for humans with the saying, "*the upmost kindness of a man is like water*, *being the most modest and gracious like water which nourishes all things without conflicts, ends up in the lowest positions and provides services without demand for a reward*".

To understand water and its various properties has always been of constant interest to mankind. Over several millennia, scientific communities have explored water as a central topic for various purposes and utilities with Archimedes' principle (287 BC–212 BC) as one early example. Truesdell (1953) and Darrigol (2005) documented in great detail the evolution of the discipline of hydrodynamics, dealing with the motion of ideal fluids as a highly hypothetical form of water, from Isaac Newton (1643–1727), Daniel Bernoulli (1700–1782) and Leonhard Euler (1707–1783) to George G. Stokes (1819–1903) and Burnett (1935, 1936).

The topic of water waves alone has attracted significant investigations, particularly from the 18th century (Stoker 1958) when many leading scientists and mathematicians joined the race to understand water waves, particularly, Joseph-Louis Lagrange (1736–1813), Seméon D. Poisson (1781–1840), Claude-Louis Navier (1785–1836), Augustin-Louis Cauchy (1789–1857), A.J.C. Barré de Saint-Venant (1797–1886), George G. Stokes (1819–1903), William Thomson (Lord Kelvin, 1824–1907), Joseph Valentin Boussinesq (1842–1929), Horace Lamb (1849–1934) and Jules Henri Poincaré (1854–1912) to list a few.

After centuries of developments by scientists, particularly physicists and mathematicians (Debler 1990), a set of general equations for fluid flow was finalized and named after two important contributors—C.L. Navier and G.G. Stokes. The Navier-Stokes equations (NSEs), discussed in Chapter 3, are fundamental equations that govern the flow of fluids, including that of water in porous media. The NSEs accommodate the viscoelasticity of the porous media, or poroviscoelasticity, and the compressibility of water to the extent of water movement in soils and aquifers.

Just like other fields of human knowledge, the pursuit of better solutions is never-ending. The high-order hydrodynamics of flow, known as Burnett hydrodynamics (Burnett 1935, 1936), is an example capable of explaining more physical mechanisms when the NSEs cease to be valid. The processes in which the high-order hydrodynamics work while the NSEs fail include phenomena such as absorption and dispersion of sound in fluids, dynamics of swarms of particles, structure of different profiles in shock waves at large Mach numbers, Couette flows, in continuum transition flows that appear around space vehicles, and flows in micro-channels (García-Colín et al. 2008).

Classic *hydrodynamics*, evolving since the 17th century, takes largely from mathematics as it deals with imaginary ideal fluids which are frictionless. Its application by experimentalists to real fluids creates the applied field of *hydraulics*. The empirical nature of hydraulics is limited in scope to water only. With the development of and interests in other forms of fluids in aeronautics, petroleum engineering and other areas in civil engineering, a broader field of study was developed—*fluid mechanics*. Fluid mechanics has three branches: *fluid statics* which is concerned with the mechanics of fluids at rest, *kinematics* which deals with velocities and streamlines without considering forces or energy, and *fluid dynamics* for the study of relations between velocities, acceleration and the forces exerted by or upon fluids in motion (Daugherty et al. 1989).

The quest for knowledge about water has created many applied fields in the modern classification of scientific and engineering disciplines. In sciences, water-related fields include fluid mechanics, hydraulics, hydrology, hydrodynamics, meteorology, oceanography, marine science, agricultural science and soil science with water as a key element. On the other hand, water-related fields in engineering comprise hydraulic engineering, irrigation and drainage engineering, marine and coastal engineering, etc.

Water has been a topic for extensive publications in various formats, and the myriad properties and aspects of water find mention in many monographs of hydrology and hydraulics and their sub-disciplines such as groundwater hydrology/hydraulics, surface water hydrology and soil hydrology.

Deformation is another aspect of soils and aquifers, for their physical properties have significant impact on civil engineering infrastructures and geological materials as well as on the environment. In particular, soil mechanics or geomechanics deals with the swelling properties of soil when its water content changes and the reciprocal changes in water pressure as a result of deformation in soil. Many reports in soil mechanics (geomechanics) can be found in parallel with publications in hydrology and hydraulics. Cauchy in 1822 and 1827 laid the foundation of the general theory of elasticity and its extension to mathematical physics (Love 1892). Cauchy's work was followed by Green in 1837 and de Saint-Venant in 1844, with six components of stress and strains investigated (Love 1892). The reports on the subsidence of geological strata first conceptualized by Pratt and Johnson (1926) in oilfields, and by Geertsma (1966) and Verruijt (1969) in aquifers resulting from the extraction of groundwater are regarded as the early examples of investigation in applied areas of geoscience. The term poroelasticity first used by Geertsma (1966) is also important for addressing this specific property of porous media (Wang 2000) in civil and petroleum engineering.

Many reports in hydrology, hydraulics and soil science dealing with soils and aquifers generally ignore the key issues of deformation and stress-strain relations, leaving such discourse for soil mechanics. The separation of soil mechanics and soil physics since the 1930s (Philip 1974) discouraged hydrology and soil science to integrate with geomechanics, making these fields apparently disconnected even though groundwater hydrologists and soil scientists deal with poroviscoelastic soils and aquifers—central topics in soil mechanics.

A weak bridge between hydrology and geomechanics was attempted in limited literature such as the works of Wang (2000), which addressed the linear poroelasticity of porous media, covering a range of issues—geomechanics (soil mechanics), hydrogeology (groundwater hydrology), petroleum engineering, the poroelasticity theory and applications based on the works of Terzaghi (1923) and Biot (1935, 1939, 1941, 1956a, b), and Biot's thermoelasticity (Biot 1941, 1956c). However, Wang's work does not discuss any aspect of the NSEs which govern the flow of water in poroelastic and thermoelastic media, thus eliminating key hydrological elements.

In terms of quantitative methods, integer partial differential equations (PDEs) have enjoyed success as the central mathematical models in hydrology, soil science, hydraulics and geomechanics, etc., for over a century since Darcy (1856) embarked on the use of differential equations (DEs) for describing water flow in porous media and Boussinesq (1904) presented PDEs for groundwater flow in unconfined aquifers.

The decade around 1990 was a turning point when fractional PDEs (fPDEs) appeared as better models, with more information about environmental processes (Lenormand 1992, Zaslavsky 1992, Compte 1997). Environmental processes such as solute transport, sediment transport and groundwater flow, etc., have been shown to be better modelled with fPDEs by Compte (1997); groundwater flow/seepage by He (1998); and solute transport in groundwater by Lenormand (1992) and Benson (1998). These developments were part of the evolution since 1974 when fractional calculus was re-launched, and monographs appeared in applied mathematics and other fields of science (Oldham and Spanier 1974, Samko et al. 1987, 1993, Miller and Ross 1993, Podlubny 1999, Kilbas et al. 2006, Hilfer 2000, Mainardi 2010, Herrmann 2011, Atanacković et al. 2014, Atangana 2018).

2. Objectives of This Book

In order to eliminate the invisible boundaries between hydrology, hydraulics, soil science and geomechanics (soil mechanics), and to address the inconsistent spectrum of mathematical models based on fPDEs in these fields, this book aims to systematically present key concepts, theories, quantitative methods and ideas centered on the application of fractional calculus in hydrology, soil science, flow in porous media and geomechanics (soil mechanics). This book aims to establish frameworks of mathematical models with concepts in fractional calculus, particularly fPDEs and fractional integral equations (fIEs), and stochastic methods such as the continuous-time random walks (CTRW) theory to water flow, solute transport and related processes.

Water flow on land is categorized as *overland flow*, water movement in unsaturated soils as *flow in unsaturated soils*, and that in saturated aquifers as *groundwater flow* (generally classified into two types—confined and unconfined aquifers). With the aforementioned goals and classification in mind, this book presents the following materials:

1. Fundamentals of mathematics in Chapter 2, dealing with concepts commonly used in fractional calculus for models and quantitative methods in hydrology and hydraulics of water flow, solute transport on land, in soils and aquifers, and soil mechanics;
2. Essential properties of soils and aquifers in the context of porous media, in Chapter 3;
3. An overview of the historical transition from quantitative methods based on integer PDEs to fractional calculus-based approach, in Chapter 4, and
4. The remaining Chapters present topics related to water flow and solute transport in *unsaturated soils* (Chapters 5, 6 and 7), *overland flow* (Chapter 8), in *saturated aquifers* (Chapters 9 and 10), and *geomechanics* (Chapter 11).

The topics in this book are central issues in *hydrology*, *soil science* and *geomechanics*, and the fundamentals, models and methodologies used for investigating water-related processes can be categorized in three parts, namely, *fundamentals*, *traditional methods* for quantification and *evolving approaches with fractional calculus*.

3. A Brief Description of Key Concepts

Soils and aquifers are porous media, the former generally unsaturated while the latter is saturated. Unsaturated soils and saturated aquifers are domains of *soil science* and *groundwater hydrology*, respectively. The land surface, both floodplains and undulating terrains, falls within the purview of *surface water hydrology*. *Porous media* of geological origin, such as soils and aquifers, are studied in geomechanics (soil mechanics), centered around the physical phenomena of deformation with viscoelastic or poroelastic properties measured by stress-strain relationships or similar terms.

Soils are either constantly unsaturated by water or variably saturated depending on the local climatic conditions such as rainfall and management options like irrigation. In most cases as reported in literature, there has been a tendency to regard soils as unsaturated porous media even though soils can be saturated. Aquifers, adjacent to the soils in the deeper strata, are physically connected to soils with varying levels of permeability for the exchange of water, solutes (a term representing chemicals, fertilizers, nutrients, microbes and other particles), gases and energy.

Porous media is the largest category of materials on the Earth. It includes a very wide range of soils and other geological strata, biological materials, and extensive types of artificial products. Soils and aquifers are major porous media of geological origin. As the biologically active and productive parts of land, soils are the most important porous media on the Earth, for they support terrestrial life. Soils are also the medium for material and energy exchanges with the atmosphere and the subsurface through a number of physical, chemical and biological processes. These processes include infiltration of water into the soil, evaporation of water from soil, percolation of infiltrated water into aquifers, and runoff on the land (hence forming streams of varying sizes, eventually leading into the oceans).

3.1 Evolution of Mathematical Models in Hydrology, Hydraulics, Soil Science, and Geomechanics Based on Fractional Calculus

Mathematical models in applied fields related to water in porous media were incepted by Darcy (1856), with a differential equation as the flux of water or its velocity in porous media, and by Boussinesq (1904), who used an entire set of PDEs for water movement in unconfined aquifers. The concept of poroelasticity since Terzaghi (1923) and Biot (1935, 1941) entered the investigations of porous media of geological origin in the 20th century. However, fractional calculus was only specifically applied to porous media after 1974 when fractional calculus was re-launched, marked by three events: publication of the first monograph on fractional calculus by Oldham and Spanier (1974); the first PhD conferred to Bertram Ross on the topic of fractional calculus; and the first *International Conference on Fractional Calculus and Its Applications* organized by Bertram Ross and held at the University of Newhaven, Connecticut in June 1974 (Miller et al. 1994).

The terminology of fractional calculus, as recorded in history, was the result of a question raised by the mathematician Marquis de L'Hôpital (1661–1704) to Gottfried Wilhelm Leibniz (1646–1716) in 1695, regarding the meaning of the differentiation of $\frac{d^n y}{dx^n}$ when $n = \frac{1}{2}$ (Kilbas et al. 2006, vii). Leibniz was unable to resolve this query of L'Hôpital's until 1819 when S.F. Lacroix proved that $\frac{d^{1/2} y(x)}{dx^{1/2}} = 2\sqrt{\frac{x}{\pi}}$ for $y(x) = x$ (Miller and Ross 1993). In 1823, Niels Henrik Abel (1802–1829) showed the result $\frac{d^{1/2} k}{dx^{1/2}} = \sqrt{\pi} f(x)$, with the integral equation $k = \int_0^x (x-t)^{-1/2} f(t)dt$ (named after him) to determine $f(x)$ for constant k (Miller and Ross 1993).

The slow evolution of fractional calculus from 1695 to 1974 saw many mathematicians and scientists in different fields applying fractional calculus to investigate various processes and phenomena. However, a complete set of fPDEs readily applicable to water flow and solute transport in soils, aquifers and closely related processes is attributed to the works of Compte (1997). This development will be detailed in Chapter 4 along with other issues.

As will be evident from Chapter 5 onwards, the order of a fractional derivative or fractional integration can be any function rather than being restricted to a fraction. It is, therefore, logical to say that fractional calculus is a generalized form of calculus, with classic integer calculus as a special case.

3.2 Developments in the Theory and Methodologies for Poroelasticity

With soil mechanics as an independent field since the 1930s (Philip 1974), the 'standard' text books and research reports on soils and aquifers in hydrology and soil science today almost ignore the deformation and stress-strain relations of porous media. An example of this fact is the Richards equation (1931) for the movement of water in soils, and many procedures dealing with various model parameter estimations.

However, with the property of porous media possessing elasticity termed as poroelasticity (Geertsma 1966, Detournay and Cheng 1993), the historical developments in elasticity, plasticity and viscoelasticity, marked by the contributions of Terzaghi (1923) and Biot (1935, 1939, 1941), signified the most important foundations relevant to flows in poroelastic media. Poroelasticity, a term first used by Geertsma (1966), according to Wang (2000), is also further named poroviscoelasticity in some cases by considering the flow of a viscous liquid in elastic porous media (Bemer et al. 2001). Both poroelasticity and poroviscoelasticity are the central issues in Chapter 11. Besides, the time-dependent deformation process described by Nutting (1921a, b) can be fundamentally treated as a creep-relaxation process that can be interpreted as a property with memory initiated by Caputo and Mainardi (1971a). The general property of thermoelastic relationships as studied by Newmann (1833) (Love 1892) and Zener (1938) constitutes more complex, yet realistic, processes of deformation and related mechanisms when poroviscoelastic materials are subjected to variable conditions.

With the introduction of the concepts of strain and stress, different methods have been developed over time to quantify the relationships of the two basic phenomena of poroelastic media (Wang 2000): *solid-to-fluid coupling* which occurs when a change in applied stress produces a change in fluid pressure or fluid mass, and *fluid-to-solid coupling* as a result of a change in the volume of the porous media due to a change in fluid pressure or fluid mass.

There are extensive literature reviews on poroviscoelastic media, some of which involve water flow and solute transport in porous media (Love 1892, Bagley and Torvik 1983, Koeller 1984, Bemer et al. 2001, Liingaard et al. 2004, Kausel 2010, Koeller 2010, Mainardi 2012, Lai et al. 2016, Sun et al. 2016).

Soil physics, since its separation from soil mechanics in the 1930s, developed its own methodologies to deal with the actual properties of soils. As outlined in section 2.8 of Chapter 3, an integral transform is used to convert the standard Cartesian coordinate in the vertical dimension to a material coordinate (represented by m) for swelling soils (Raats 1965, Raats and Klute 1968, Smiles and Rosenthal 1968, Philip 1969b, Philip and Smiles 1969). With this approach for swelling-shrinking soils, the material coordinate is valid for vertically deforming soils by neglecting the horizontal expansion of the soil resulting from an increase in the water content of swelling soils. This simplification allows deformation to be analyzed with void ratio as the variable which depends on the moisture content in the soil. Similar to the development of ideas for elasticity and deformation, more complicated factors like the thermal effect and time-dependent processes or processes with memory, etc., can also be introduced.

As Mainardi (2010, 26) and Mainardi and Spada (2011) showed, linear elasticity can be quantitatively related as reciprocal relations which have been observed in the field (Hsieh 1996) and are used for estimating aquifer parameters (Burbey 2001). fPDEs have also been developed to investigate water flow in soils by incorporating swelling-shrinking properties of soils (Su 2010, 2012, 2014). These topics are discussed in Chapters 5, 6 and 7.

3.3 Hydrology, Hydraulics, Soil Science, Geomechanics (Soil Mechanics) and Their Relevance to Environmental Issues

Despite its irreplaceable role in all the sectors of society and for sustaining life on Earth, water is, however, often taken for granted. The continual worldwide pollution of soils and land, water bodies and oceans is an example of this ignorance and has been highlighted in numerous reports by FAO (2015), UNEP (2017) and UNESCO (2018).

Solutes in water and in porous media, collectively referring to a number of materials like ions, microbes, natural or artificial particles and pollutants or contaminants of various forms, are central to the issues of environmental and health concerns. The integral analysis of water movement, solute transport and related processes in deforming porous media, with fPDEs and fIEs, is a major focus of this book. To this end, the objective here is to achieve an improved understanding and quantification of water-related processes in soils and aquifers as well as on the surface to sustainably manage the limited resources of water and land.

4. Notation in the Book

Throughout the book, mathematical symbols have been defined independently in each chapter, thus a small number of symbols having different definitions in different chapters. I have tried to ensure consistency in the definition of symbols within each chapter, except in a few cases wherein the original equations have been preserved with the corresponding specific symbols.

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