Geosystems Mathematics

Series Editors
Willi Freeden
Kaiserslautern, Germany

M. Zuhair Nashed
Orlando, Florida, USA

Birkhäuser

This series provides an ideal frame and forum for the publication of mathematical key technologies and their applications to geo-scientific and geo-related problems. Current understanding of the highly complex system Earth with its interwoven subsystems and interacting physical, chemical, and biological processes is not only driven by scientific interest but also by the growing public concern about the future of our planet, its climate, its environment, and its resources. In this situation mathematics provides concepts, tools, methodology, and structures to characterize, model, and analyze this complexity at various scales. Modern high speed computers are increasingly entering all geo-disciplines. Terrestrial, airborne as well as spaceborne data of higher and higher quality become available. This fact has not only influenced the research in geosciences and geophysics, but also increased relevant mathematical approaches decisively as the quality of available data was improved.

Geosystems Mathematics showcases important contributions and helps to promote the collaboration between mathematics and geo-disciplines. The closely connected series *Lecture Notes in Geosystems Mathemactics and Computing* offers the opportunity to publish small books featuring concise summaries of cutting-edge research, new developments, emerging topics, and practical applications. Also PhD theses may be evaluated, provided that they represent a significant and original scientific advance.

More information about this series at http://www.springer.com/series/13389

Nicolae Suciu

Diffusion in Random Fields

Applications to Transport in Groundwater

Birkhäuser

Nicolae Suciu
Department of Mathematics
Friedrich-Alexander University
of Erlangen-Nürnberg
Erlangen, Germany

Tiberiu Popoviciu Institute
of Numerical Analysis
Cluj-Napoca Branch
of the Romanian Academy
Cluj-Napoca, Romania

ISSN 2510-1544 ISSN 2510-1552 (electronic)
Geosystems Mathematics
ISBN 978-3-030-15080-8 ISBN 978-3-030-15081-5 (eBook)
https://doi.org/10.1007/978-3-030-15081-5

Mathematics Subject Classification (2010): 60J60, 60G60, 65C10, 65M75, 65C05, 76S05, 86A05

This book is published under the imprint Birkhäuser, www.birkhauser-science.com by the registered company Springer Nature Switzerland AG.
The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

In memory of Călin Vamoş (1955–2017)

Preface

The aim of this book is to provide an accessible and self-consistent theory of diffusion in random velocity fields together with robust numerical simulation approaches. The focus is on transport processes in natural porous media, with applications to contaminant transport in groundwater.

Stochastic modeling has been a leading paradigm in studies of complex systems for several decades. Random media, random environments, or random fields are central topics for thousands of research papers in physics, technology, geophysics, and life sciences. For instance, a search for the topic "random media" (with quotes) in Web of Science (seen online in January 2019) returned 5030 results with 18.64 citations per item in the last two decades, with a strong increasing trend. A similar dynamics (4466 results with 15.54 citations per item) shows for the same period the topic "groundwater contamination," which is one of the investigation directions where the "randomness" paradigm is intensively used.

Mathematical models of transport in random environments (e.g., continuous diffusion processes with random coefficients or random walks with random jump probabilities) are often used for phenomena which are not reproducible experimentally under macroscopically identical conditions or in cases where the incomplete knowledge of the physical parameters precludes deterministic descriptions. To the first class belongs the turbulence, characterized by an intrinsic randomness, which is modeled by random velocity fluctuations. Also in plasma physics the turbulent state of the system of charged particles is described by random electric potentials and magnetic fields. Transport in groundwater belongs to the second class. The way randomness enters modeling in hydrogeology is through stochastic parameterizations of incompletely known hydraulic conductivity fields which induce random Darcy velocity fields.

A common feature of transport processes in random environments is the apparent increase of the diffusion coefficients with the scale of observation. In hydrogeology, the increase from Darcy scale to laboratory and to field scale of the diffusion coefficients inferred from measurements through different approaches (by fitting concentrations with solutions of advection-diffusion equations, by computing spatial moments of tracer concentrations, or by analysis of concentration series recorded at different travel distances from the source) has been called “scale effect.” Similar scale dependence characterizes the so-called running diffusion coefficient in plasma physics and the “turbulent diffusivity” in turbulence.

Another characteristic of transport in random media is the presence of various memory effects associated with the departure of the transport process from a genuine Gaussian diffusion. In turbulence and in plasma physics, memory effects manifested by non-Markovian evolution were explicitly associated with the stochastic nature of the environment. In the frame of stochastic subsurface hydrology, the departure from Fickian, linear-time behavior of the second moment of the solute plume can be interpreted as a memory effect. This type of memory effect is usually associated with Markovian diffusion processes and is omnipresent in stochastic models of transport in groundwater. The prototype memory-free process is the Wiener process with independent increments. Therefore, a direct quantification of such memory effects is provided by correlations of increments of the transport process.

The groundwater is contained in aquifer systems consisting of spatially heterogeneous hydrogeological formations. The scarcity of direct measurements of their hydraulic conductivity is compensated by spatial interpolations and correlations. Based on such empirical models, the hydraulic conductivity is further modeled by space random functions. The groundwater flow driven by piezometric pressure gradients is usually modeled by Darcy’s law, and the randomness of the hydraulic conductivity induces the randomness of the flow velocity. Contaminant solutes are transported by advection, are diluted by diffusion and hydrodynamic dispersion, and undergo various chemical reactions. Under simplifying assumptions, also supported by experiments, the hydrodynamic dispersion is approximated by a Gaussian diffusion and summing up the molecular diffusion at the pore scale one arrives at a local-scale diffusive model with diffusive flux governed by Fick’s law. Hence, the primary mechanism governing the fate of contaminants in groundwater can be described as a diffusion in random velocity fields.

For fixed realizations of the random velocity field, concentrations and transition probability densities of the diffusion process are governed by parabolic partial differential equations local in time and space. However, in case of statistically nonhomogeneous velocity fields, theoretical investigations and numerical simulations show that the evolution of the ensemble average concentration is non-Fickian and has to be described by integro-differential equations nonlocal in both time and space. A model nonlocal in time but local in space of the ensemble average concentration is the “continuous time random walk” process, with uncorrelated polydisperse features consisting of a random walk with waiting times uniformly sampled from a probability distribution. Non-locality also occurs in modeling the local dispersion if the hydraulic parameters of the medium display a fractal structure. Since nonlocal and non-Fickian behavior may arise from either normal or anomalous local-scale diffusion models, it is difficult to extract information on the true nature of the stochastic transport process from experiments. Moreover, if the hydraulic conductivity and the velocity field are characterized by power-law correlations, the model of diffusion in random fields naturally leads to anomalous diffusive behavior of the transport process. Thus, diffusion in random velocity fields remains competitive with respect to other models of non-Fickian behavior.

Unlike models of ensemble-averaged observables of the transport process, the model of diffusion in random fields allows straightforward Monte Carlo (MC) estimates of prediction errors and ergodicity assessments. They can be obtained by comparing results for fixed realizations of the random field, corresponding to the observed transport process, to their ensemble averages. Last but not least, the model of diffusion in random velocity fields is formulated as a Fokker–Planck equation with random coefficients which is appropriate and facilitates the development of methods similar to those used in turbulence studies for the probability density function (PDF) of the random concentration.

The Fokker–Planck structure of the model equations is of great importance in numerical simulations. The solution of the Fokker–Planck equation is essentially the probability density of an Itô diffusion process. This property provides the basis for constructing various "particle methods," such as random walks on lattices or grid-free "particle tracking" (PT) approaches. The latter are actually solutions of Itô stochastic differential equations. Particle densities estimated from ensembles of random walk or PT solutions provide the numerical solution of the Fokker–Planck equation. These approaches are generalized by the "global random walk" (GRW) algorithm. It consists of a superposition of many weak Euler schemes for the Itô equation projected on a regular lattice. The associated system of computational particles evolves globally, by simultaneous jumps of all the particles from a lattice site to neighboring sites according to the random walk rule.

The book consists of seven chapters. Following the introductory Chap. 1, which presents an overview of the problems and the model equations, and Chap. 2, which introduces the basic notions of random variables, random functions, and diffusion processes, Chap. 3 is devoted to numerical simulations of diffusion processes and GRW algorithms. Chapter 4 presents the mathematical model of diffusion in random fields in relation to applications to stochastic modeling in subsurface hydrology. Memory effects and ergodicity issues are investigated by MC simulations in Chap. 5. A mathematical frame of PDF approaches and numerical solutions of PDF evolution equations obtained with the GRW algorithm are presented in Chap. 6. Chapter 7 concludes the book by discussing the relation between model and measurement scales and introduces a new approach which accounts for measurement scale through spatiotemporal averages of GRW solutions. Some technical details are deferred to Appendices A–F.

The moderate level of difficulty of the presentation and the minimum necessary information on stochastic processes provided in the first three chapters make the book accessible to readers with an undergraduate background in engineering or physics. More challenging issues presented in Chaps. 4–7, such as the correlation structure of the process of diffusion in random fields, relation between memory effects and ergodic properties, and derivation and parameterizations of PDF equations, could be of interest for researchers with an advanced mathematical and engineering background and could serve as the basis for further developments in stochastic modeling of groundwater systems.

Nürnberg, Germany
January 2019

Nicolae Suciu

Acknowledgements

Parts of this book present results obtained during several research projects supported by the Deutsche Forschungsgemeinschaft–Germany under Grants SU 415/1-1, and SU 415/1-2, SU 415/2-1, SU 415/4-1. Massive Monte Carlo simulations have been supported by the Jülich Supercomputing Centre–Germany as part of the Project JICG41. Fruitful cooperation with colleagues from Tiberiu Popoviciu Institute of Numerical Analysis of the Romanian Academy, Agrosphere Institute of the Research Centre Jülich, Chair of Applied mathematics 1 of the Friedrich-Alexander University Erlangen-Nürnberg, Helmholtz Centre for Environmental Research—UFZ, Leipzig, and the Department of Mathematics of the University of Bergen is gratefully acknowledged.

Contents