In his forward-looking paper [374] at the conference “Mathematics Towards the Third Millennium,” our esteemed colleague at Brown University Prof. David Mumford argued that “…stochastic models and statistical reasoning are more relevant to i) the world, ii) to science and many parts of mathematics and iii) particularly to understanding the computations in our mind, than exact models and logical reasoning.” Deterministic modeling and corresponding simulations are computationally much more manageable than stochastic simulations, but they also offer much less, i.e., a single point in the “design space” instead of a “sphere” of possible solutions that reflect the various random (or not) perturbations of the physical or biological problem we study.

In the last twenty years, three-dimensional simulations of physical and biological phenomena have gone from an exception to the rule, and they have been widely adopted in Computational Science and Engineering (CSE). This more realistic approach to simulating physical phenomena together with the continuing fast increase of computer speeds has also led to the desire in performing more ambitious and even more realistic simulations with multiscale physics. However, not all scales can be modeled directly, and stochastic modeling has been used to account for the un-modeled physics. In addition, there is a fundamental need to quantify the uncertainty of large-scale simulations, and this has led to a new emerging field in CSE, namely that of Uncertainty Quantification or UQ. Hence, computational scientists and engineers are interested in endowing their simulations with “error bars” that reflect not only numerical discretization errors but also uncertainties associated with unknown precise values of material properties, ill-defined or even unknown boundary conditions, or uncertain constitutive laws in the governing equations. However, performing UQ taxes the computational resources greatly, and hence the selection of the proper numerical method for stochastic simulations is of paramount importance, in some sense much more important than selecting a numerical method for deterministic modeling.
The most popular simulation method for stochastic modeling is the Monte Carlo method and its various extensions, but it requires a lot of computational effort to compute thousands and often millions of sample paths required to obtain certain statistics of the quantity of interest. Specifically, Monte Carlo methods are quite general, but they suffer from slow convergence so they are usually employed in conjunction with some variance reduction techniques to produce satisfactory accuracy in practice. More recently and for applications that employ stochastic models with color noise, deterministic integration methods in random space have been used with great success as they lead to high accuracy, especially for a modest number of uncertain parameters. However, they are not directly applicable to stochastic partial differential equations (SPDEs) with temporal white noise, since their solutions are usually non-smooth and would require a very large number of random variables to obtain acceptable accuracy.

**Methodology.** For linear SPDEs, we can still apply deterministic integration methods by exploiting the linear property of these equations for a long-time numerical integration. This observation has been made in [315] for Zakai-type equations, where a recursive Wiener chaos method was developed. In this book, we adopt this idea and we further formulate a recursive strategy to solve linear SPDEs of general types using Wiener chaos methods and stochastic collocation methods in conjunction with sparse grids for efficiency. In order to apply these deterministic integration methods, we first truncate the stochastic processes (e.g., Brownian motion) represented by orthogonal expansions. In this book, we show that the orthogonal expansions can lead to higher-order schemes with proper time discretization when Wiener chaos expansion methods are employed. However, we usually keep only a small number of truncation terms in the orthogonal expansion of Brownian motion to efficiently use deterministic integration methods for temporal noise. For spatial noise, the orthogonal expansion of Brownian motions leads to higher-order methods in both random space and physical space when the solutions to the underlying SPDEs are smooth.

The framework we use is the Wong-Zakai approximation and Wiener chaos expansion. Wiener chaos expansion is associated with the Ito-Wick product which was used intensively in [223]. The methodology and the proofs are introduced in [315] and in some subsequent papers by Rozovsky and his collaborators. In this framework, we are led to systems of deterministic partial differential equations with unknowns being the Wiener chaos expansion coefficients, and it is important to understand the special structure of these linear systems. Following another framework, such as viewing the SPDEs as infinite-dimensional stochastic differential equations (SDEs), admits a ready application of numerical methods for SDEs. We emphasize that there are multiple points of view for treating SPDEs and accordingly there are many views on what are proper numerical methods for SPDEs. However, irrespective of such views, the common difficulty remains: the solutions are typically
very rough and do not have first-order derivatives either in time or in space. Hence, no high-order (higher than first-order) methods are known except in very special cases.

Since the well-known monographs on numerical SDEs by Kloeden & Platen (1992) [259], Milstein (1995) [354], and Milstein & Tretyakov (2004) [358], numerical SPDEs with white noise have gained popularity, and there have been some new books on numerical SPDEs available, specifically:

- The book by Jentzen & Kloeden (2011) [251] on the development of stochastic Taylor’s expansion for mild solutions to stochastic parabolic equations and their application to numerical methods.
- The book by Kruse (2014) [277] on numerical methods in space and time for semi-linear parabolic equations driven by space-time noise addressing strong ($L^p$ or mean-square) and weak (moments) sense of convergence.

For numerical methods of stochastic differential equations with color noise, we refer the readers to [294, 485]. On the theory of SPDEs, there are also some new developments, and we refer the interested readers to the book [36] covering amplitude equations for nonlinear SPDEs and to the book [119] on homogenization techniques for effective dynamics of SPDEs.

**How to use this book.** This book can serve as a reference/textbook for graduate students or other researchers who would like to understand the state-of-the-art of numerical methods for SPDEs with white noise.

Reading this book requires some basic knowledge of probability theory and stochastic calculus, which are presented in Chapter 2 and Appendix A. Readers are also required to be familiar with numerical methods for partial differential equations and SDEs in Chapter 3 before further reading. The reader can also refer to Chapter 3 for MATLAB implementations of test problems. More MATLAB codes for examples in this book are available upon request. For those who want to take a glance of numerical methods for stochastic partial differential equation, they are encouraged to read a review of these methods presented in Chapter 3. Exercises with hints are provided in most chapters to nurture the reader’s understanding of the presented materials.

**Part I. Numerical stochastic ordinary differential equations.** We start with numerical methods for SDEs with delay using the Wong-Zakai approximation.
and finite difference in time in Chapter 4. The framework of Wong-Zakai approximation is used throughout the book. If the delay time is zero, we then recover the standard SDEs. We then discuss how to deal with strong nonlinearity and stiffness in SDEs in Chapter 5.

**Part II. Temporal white noise.** In Chapters 6–8, we consider SPDEs as PDEs driven by white noise, where discretization of white noise (Brownian motion) leads to PDEs with smooth noise, which can then be treated by numerical methods for PDEs. In this part, recursive algorithms based on Wiener chaos expansion and stochastic collocation methods are presented for linear stochastic advection-diffusion-reaction equations. Stochastic Euler equations in Chapter 9 are exploited as an application of stochastic collocation methods, where a numerical comparison with other integration methods in random space is made.

**Part III. Spatial white noise.** We discuss in Chapter 10 numerical methods for nonlinear elliptic equations as well as other equations with additive noise. Numerical methods for SPDEs with multiplicative noise are discussed using the Wiener chaos expansion method in Chapter 11. Some SPDEs driven by non-Gaussian white noise are discussed, where some model reduction methods are presented for generalized polynomial chaos expansion methods.

We have attempted to make the book self-contained. Necessary background knowledge is presented in the appendices. Basic knowledge of probability theory and stochastic calculus is presented in Appendix A. In Appendix B, we present some semi-analytical methods for SPDEs. In Appendix C, we provide a brief introduction to Gauss quadrature. In Appendix D, we list all the conclusions we need for proofs. In Appendix E, we present a method to compute convergence rate empirically.

MATLAB codes accompanying this book are available at the following website:


**Acknowledgments.** This book is dedicated to Dr. Fariba Fahroo who with her quiet and steady leadership at AFOSR and DARPA and with her generous advocacy and support has established the area of uncertainty quantification and stochastic modeling as an independent field, indispensable in all areas of computational simulation of physical and biological problems.

This book is based on our research through collaboration with Professor Boris L. Rozovsky at Brown University and Professor Michael V. Tretyakov at the University of Nottingham. We are indebted to them for their valuable advice. Specifically, Chapters 6, 7, and 8 are based on collaborative research with them. Chapter 5 is also from a collaboration with Professor Michael V. Tretyakov. We would also like to thank Professor Wanrong Cao at Southeast University for providing us numerical results in Chapter 4 and Professor Guang Lin at Purdue University and Dr. Xiu Yang at Pacific Northwest National Laboratory for providing their code for Chapter 9.
The research of this book was supported by OSD/MURI grant FA9550-09-1-0613, NSF/DMS grant DMS-0915077, NSF/DMS grant DMS-1216437, and ARO and NIH grants and also by the Collaboratory on Mathematics for Mesoscopic Modeling of Materials (CM4) which is sponsored by DOE. The first author was also supported by a start-up funding at Worcester Polytechnic Institute during the writing of the book.

Worcester, MA, USA  Zhongqiang Zhang
Providence, RI, USA  George Em Karniadakis
Numerical Methods for Stochastic Partial Differential Equations with White Noise
Zhang, Z.; Karniadakis, G.E.
2017, XV, 394 p. 36 illus., 34 illus. in color. With online files/update., Hardcover
ISBN: 978-3-319-57510-0