Spectral Methods for Uncertainty Quantification

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O.P. Le Maître · O.M. Knio

Spectral Methods for Uncertainty Quantification

With Applications to Computational Fluid Dynamics

Springer

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To the Ladies, certainly,
Marie-Christine & May

Preface

This book deals with the application of spectral methods to problems of uncertainty propagation and quantification in model-based computations. It specifically focuses on computational and algorithmic features of these methods which are most useful in dealing with models based on partial differential equations, with special attention to models arising in simulations of fluid flows. Implementations are illustrated through applications to elementary problems, as well as more elaborate examples selected from the authors' interests in incompressible vortex-dominated flows and compressible flows at low Mach numbers.

Spectral stochastic methods are probabilistic in nature, and are consequently rooted in the rich mathematical foundation associated with probability and measure spaces. Despite the authors' fascination with this foundation, the discussion only alludes to those theoretical aspects needed to set the stage for subsequent applications. The book is authored by practitioners, and is primarily intended for researchers or graduate students in computational mathematics, physics, or fluid dynamics. The book assumes familiarity with elementary methods for the numerical solution of time-dependent, partial differential equations; prior experience with spectral methods is naturally helpful though not essential. Full appreciation of elaborate examples in computational fluid dynamics (CFD) would require familiarity with key, and in some cases delicate, features of the associated numerical methods. Besides these shortcomings, our aim is to treat algorithmic and computational aspects of spectral stochastic methods with details sufficient to address and reconstruct all but those highly elaborate examples.

This book is composed of 10 chapters. Chapter 1 discusses the relevance and (ever increasing) role of uncertainty propagation and quantification in model-based predictions. This is followed with brief comments on various approaches used to deal with model data uncertainties, focusing in particular on a probabilistic framework that forms the foundation for subsequent discussion. The remaining nine chapters are divided into two parts.

Part I (Chaps. 2–6) focuses on basic formulations and mechanics, providing diverse illustrations based on elementary examples. Chapter 2 discusses fundamentals of spectral expansions of random parameters and processes. Treated in detail are the classical concepts underlying Karhunen-Loève (KL) expansions, homogeneous chaos, and polynomial chaos (PC). An outline is also provided of the application of these concepts to the representation of uncertain model data, and to the representation of the corresponding uncertain model outputs. Chapter 3 discusses so-called non-intrusive spectral methods of uncertainty propagation. These resemble collocation methods used in the numerical solution of PDEs, and are termed non-intrusive since they generally do not require modification of existing or legacy simulation codes. The discussion covers several approaches falling within this class of spectral methods, including stochastic quadratures, as well as cubature and regression methods. In Chap. 4, we discuss Galerkin (intrusive) approaches to uncertainty propagation, focusing in particular on weak formulations of stochastic problems involving data uncertainty. Stochastic basis function expansions are introduced, and the setup of the resulting stochastic problem is discussed in detail. Special attention is paid to the estimation of nonlinearities, and a brief outline of solution methods is provided. Chapter 5 provides detailed illustration of the implementation of PC methods to simple problems, namely through application to transient diffusion equations in two space dimensions, and to the steady Burgers equation in one space dimension. Chapter 6 then provides several examples illustrating the application of various approaches introduced in Chaps. 3 and 4 to flows governed by the time-dependent Navier-Stokes equations. Examples include incompressible flows, variable-density flows at low-Mach-number, and electrokinetically driven flows.

Part II (Chaps. 7–10) focuses exclusively on Galerkin methods, and deals with more advanced topics, more recent developments, or more elaborate applications. Chapter 7 discusses the application of specialized solution methods that are of general interest in stochastic flow computations. These include methods for finding stochastic stationary flow solutions, stochastic multigrid solvers, and a brief discussion of pre-conditioning and Krylov methods for the resolution of large systems of linear equations arising in Galerkin projections. Chapter 8 deals with generalized spectral representation concepts, particularly wavelet and multiwavelet representations, as well as multi-resolution analysis of stochastic problems. The applicability of these schemes to problems exhibiting discontinuous dependence on model data is emphasized, and is illustrated using applications to simple dynamical problems and to flow computations. Chapter 9 deals with adaptive representations, stochastic domain decomposition techniques, stochastic error estimation and refinement, and reduced basis approximations. New challenges, open questions, and closing remarks are mentioned in Chap. 10.

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