Volume 8

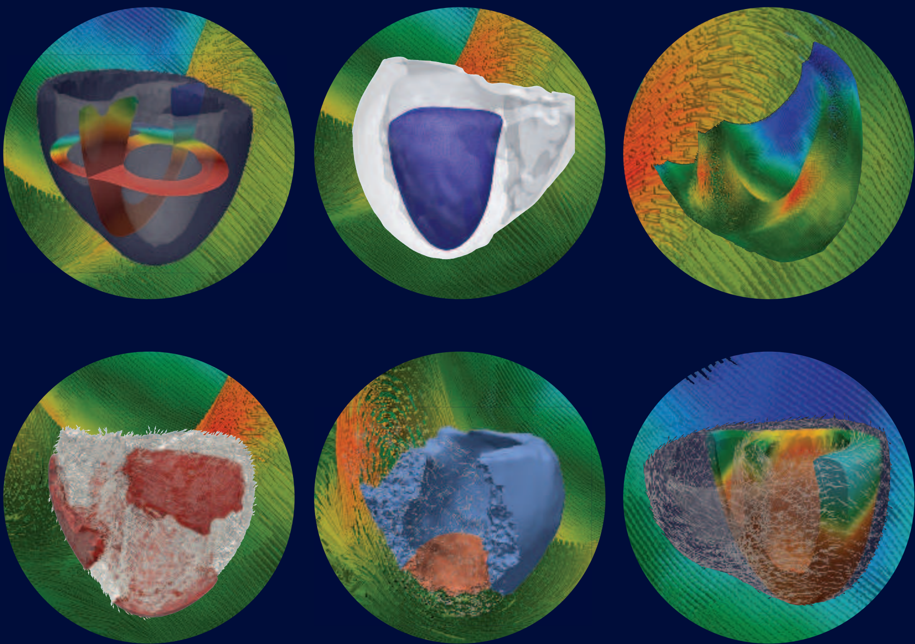
Numerical Models for Differential Problems

Second Edition

Alfio Quarteroni

MS&A

Modeling, Simulation & Applications



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To Fulvia, Silvia and Marzia

Preface to the second edition

Differential equations (DEs) are the foundation on which many mathematical models for real-life applications are built. These equations can seldom be solved in 'closed' form: in fact, the exact solution can rarely be characterized through explicit, and easily computable, mathematical formulae. Almost invariably one has to resort to appropriate numerical methods, whose scope is the approximation (or discretization) of the exact differential model and, hence, of the exact solution.

This is the second edition of a book that first appeared in 2009. It presents in a comprehensive and self-contained way some of the most successful numerical methods for handling DEs, for their analysis and their application to classes of problems that typically show up in the applications.

Although we mostly deal with partial differential equations (PDEs), both for steady problems (in multiple space dimensions) and time-dependent problems (with one or several space variables), part of the material is specifically devoted to ordinary differential equations (ODEs) for one-dimensional boundary-value problems, especially when the discussion is interesting in itself or relevant to the PDE case.

The primary concern is on the finite-element (FE) method, which is the most popular discretization technique for engineering design and analysis. We also address other techniques, albeit to a lesser extent, such as finite differences (FD), finite volumes (FV), and spectral methods, including further *ad-hoc* methods for specific types of problems. The comparative assessment of the performance of different methods is discussed, especially when it sheds light on their mutual interplay.

We also introduce and analyze numerical strategies aimed at reducing the computational complexity of differential problems: these include operator-splitting and fractional-step methods for time discretization, preconditioning, techniques for grid adaptivity, domain decomposition (DD) methods for parallel computing, and reduced-basis (RB) methods for solving parametrized PDEs efficiently.

Besides the classical elliptic, parabolic and hyperbolic linear equations, we treat more involved model problems that arise in a host of applicative fields: linear and nonlinear conservation laws, advection-diffusion equations with dominating advection, Navier-Stokes equations, saddle-point problems and optimal-control problems.

Here is the contents' summary of the various chapters.

Chapter 1 briefly surveys PDEs and their classification, while Chapter 2 introduces the main notions and theoretical results of functional analysis that are extensively used throughout the book.

In Chapter 3 we illustrate boundary-value problems for elliptic equations (in one and several dimensions), present their weak or variational formulation, treat boundary conditions and analyze well-posedness. Several examples of physical interest are introduced.

The book's first cornerstone is Chapter 4, where we formulate Galerkin's method for the numerical discretization of elliptic boundary-value problems and analyze it in an abstract functional setting. We then introduce the Galerkin FE method, first in one dimension, for the reader's convenience, and then in several dimensions. We construct FE spaces and FE interpolation operators, prove stability and convergence results and derive several kinds of error estimates. Eventually, we present grid-adaptive procedures based on either *a priori* or *a posteriori* error estimates.

The numerical approximation of parabolic problems is explained in Chapter 5: we begin with semi-discrete (continuous in time) Galerkin approximations, and then consider fully-discrete approximations based on FD schemes for time discretization. For both approaches stability and convergence are proven.

Chapters 6, 7 and 8 are devoted to the algorithmic features and the practical implementation of FE methods. More specifically, Chapter 6 illustrates the main techniques for grid generation, Chapter 7 surveys the basic algorithms for the solution of ill-conditioned linear algebraic systems that arise from the approximation of PDEs, and Chapter 8 presents the main operational phases of a FE code, together with a complete working example.

The basic principles underlying finite-volume methods for the approximation of diffusion-transport-reaction equations are discussed in Chapter 9. FV methods are commonly used in computational fluid dynamics owing to their intrinsic, built-in conservation properties.

Chapter 10 addresses the multi-faceted aspects of spectral methods (Galerkin, collocation, and the spectral-element method), analyzing thoroughly the reasons for their superior accuracy properties.

Galerkin discretization techniques relying on discontinuous polynomial subspaces are the subject of Chapter 11. We present, more specifically, the discontinuous Galerkin (DG) method and the mortar method, together with their use in the context of finite elements or spectral elements.

Chapter 12 focuses on singularly perturbed elliptic boundary-value problems, in particular diffusion-transport equations and diffusion-reaction equations, with small diffusion. The exact solutions to this type of problems can exhibit steep gradients in tiny subregions of the computational domains, the so-called internal or boundary layers. A great deal of attention is paid to stabilization techniques meant to prevent the on-rise of oscillatory numerical solutions. Upwinding techniques are discussed for FD approximations, and their analogy with FE with artificial diffusion is analyzed. We introduce and discuss other stabilization approaches in the FE context, as well, which lead to the sub-grid generalized Galerkin methods, the Petrov-Galerkin methods and Galerkin's Least-Squares method.

The ensuing three chapters form a thematic unit focusing on the approximation of first-order hyperbolic equations. Chapter 13 addresses classical FD methods. Stability is investigated using both the energy method and the Von Neumann analysis. Using the latter we also analyze the properties of dissipation and dispersion featured by a numerical scheme. Chapter 14 is devoted to spatial approximation by FE methods, including the DG methods and spectral methods. Special emphasis is put on characteristic compatibility conditions for the boundary treatment of hyperbolic systems. A very quick overview of the numerical approximation of nonlinear conservation laws is found in Chapter 15. Due to the relevance of this particular topic the interested reader is advised to consult the specific monographs mentioned in the references.

In Chapter 16 we discuss the Navier-Stokes equations for incompressible flows, plus their numerical approximation by FE, FV and spectral methods. A general stability and convergence theory is developed for spatial approximation of saddle-point problems, which comprises strategies for stabilization. Next we propose and analyze a number of time-discretization approaches, among which finite differences, characteristic methods, fractional-step methods and algebraic factorization techniques. Special attention is devoted to the numerical treatment of interfaces in the case of multiphase flows.

Chapter 17 discusses the issue of optimal control for elliptic PDEs. The problem is first formulated at the continuous level, where conditions of optimality are obtained using two different methods. Then we address the interplay between optimization and numerical approximation. We present several examples, some of them elementary in character, others involving physical processes of applicative relevance.

Chapter 18 regards domain-decomposition methods. These techniques are specifically devised for parallel computing and for the treatment of multiphysics' PDE problems. The families of Schwarz methods (with overlapping subdomains) and Schur methods (with disjoint subdomains) are illustrated, and their convergence properties of optimality (grid invariance) and scalability (subdomain-size invariance) studied. Several examples of domain-decomposition preconditioners are provided and tested numerically.

Finally, in Chapter 19 we introduce the reduced-basis (RB) method for the efficient solution of PDEs. RB methods allow for the rapid and reliable evaluation of input/output relationships in which the output is expressed as a functional of a field variable that is the solution of a parametrized PDE. Parametrized PDEs model several processes relevant in applications such as steady and unsteady transfer of heat or mass, acoustics, solid and fluid mechanics, to mention a few. The input-parameter vector variously characterizes the geometric configuration of the domain, physical properties, boundary conditions or source terms. The combination with an efficient *a posteriori* error estimate, and the splitting between offline and online calculations, are key factors for RB methods to be computationally successful.

Many important topics that would have deserved a proper treatment were touched only partially (in some cases completely ignored). This depends on the desire to offer a reasonably-sized textbook on one side, and our own experience on the other. The list of notable omissions includes, for instance, the approximation of equations for the structural analysis and the propagation of electromagnetic waves. Detailed studies can be found in the references' specialized literature.

This text is intended primarily for graduate students in Mathematics, Engineering, Physics and Computer Science and, more generally, for computational scientists. Each chapter is meant to provide a coherent teaching unit on a specific subject. The first eight chapters, in particular, should be regarded as a comprehensive and self-contained treatise on finite elements for elliptic and parabolic PDEs. Chapters 9–16 represent an advanced course on numerical methods for PDEs, while the last three chapters contain more subtle and sophisticated topics for the numerical solution of complex PDE problems.

This work has been used as a textbook for graduate-level courses at the Politecnico di Milano and the École Polytechnique Fédérale de Lausanne. We would like to thank the many people – students, colleagues and readers – who contributed, at various stages and in many different ways, to its preparation and to the improvement of early drafts. A (far from complete) list includes Paola Antonietti, Luca Dedé, Marco Discacciati, Luca Formaggia, Loredana Gaudio, Paola Gervasio, Andrea Manzoni, Stefano Micheletti, Nicola Parolini, Anthony T. Patera, Luca Pavarino, Simona Perotto, Gianluigi Rozza, Fausto Saleri, Benjamin Stamm, Alberto Valli, Alessandro Veneziani, and Cristoph Winkelmann. Special thanks go to Luca Paglieri for the technical assistance, to Francesca Bonadei of Springer for supporting this project since its very first Italian edition, and, last but not least, to Silvia Quarteroni for the translation from Italian and to Simon G. Chiossi for the linguistic revision of the second edition.

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