# Preface

This book deals with numerical methods for solving partial differential equations (PDEs) coupling advection, diffusion and reaction terms, with a focus on time-dependency. A combined treatment is presented of methods for hyperbolic problems, thereby emphasizing the one-way wave equation, methods for parabolic problems and methods for stiff and non-stiff ordinary differential equations (ODEs). With regard to time-dependency we have attempted to present the algorithms and the discussion of their properties for the three different types of differential equations in a unified way by using semi-discretizations, i.e., the method of lines, whereby the PDE is transformed into an ODE by a suitable spatial discretization. In addition, for hyperbolic problems we also discuss discretizations that use information based on characteristics. Due to this combination of methods, this book differs substantially from more specialized textbooks that deal exclusively with numerical methods for either PDEs or ODEs. We treat integration methods suitable for both classes of problems.

This combined treatment offers a clear advantage. On the one hand, in the field of numerical ODEs highly valuable methods and results exist which are of practical use for solving time-dependent PDEs, something which is often not fully exploited by numerical PDE researchers. Although many problems can be solved by Euler's method or the Crank-Nicolson method, better alternatives are often available which can significantly reduce the computational effort needed to solve practical problems. On the other hand, many numerical ODE researchers are unaware of the vast amount of highly interesting results on discretization methods for PDEs. Moreover, when solving PDEs, discretizations in space and time have to be matched, and different spatial discretizations may require different temporal discretizations. It is our hope that this book bridges these gaps, if not fully, then at least partially.

With regard to applications our aim has been to present material specifically directed at solving so-called transport-chemistry problems, i.e., problems where the transport part is based on advection and diffusion processes and the chemistry part on chemical reaction processes modelled by ordinary differential equations. Such transport-chemistry problems are frequently used in environmental modelling, notably in connection with pollution of atmospheric air, surface water and groundwater. Similar problem types are also found in mathematical biology, for instance with chemo-taxis problems that are used to study bacterial growth, tumour growth and related biochemical phenomena. Hence throughout the book our dependent variables mostly represent concentrations of chemical species, and we therefore give considerable attention to monotonicity and positivity properties of numerical schemes, i.e., to the question how to prevent spurious, negative numerical concentrations associated with spurious temporal and spatial oscillations, the plague of many discretization methods for differential equations with dominating hyperbolic terms.

The focus on advection-diffusion-reaction problems enabled us to keep the size of the text within reasonable limits. As a consequence, however, for certain important classes of PDEs, like the Maxwell and Navier-Stokes equations, only some aspects are touched. Moreover, the main focus in this book is on time-dependency. Spatial discretizations are obtained by finite differences or finite volumes, and, to a lesser degree, by finite elements. Spectral methods and their variants are not treated, nor are elliptic problems and the associated, specialized numerical linear algebra solvers.

The book has five chapters of which the first gives an introduction to the wide field of numerical solution of evolutionary PDEs and to the more specialized material presented in later chapters. This first chapter is written primarily for readers and students of applied and numerical mathematics and the exact sciences with little numerical training; this chapter contains exercises in footnotes. Once the first chapter is digested, the remaining four should be accessible. More experienced readers and students could skip most of Chapter I and concentrate on the more specialized subjects of Chapters II – V, dealing with time integration methods, advection-diffusion discretizations, splitting methods and stabilized explicit Runge-Kutta methods. These subjects have been chosen because of their practical relevance for solving advection-diffusion-reaction problems. But they obviously also reflect our personal taste and research history.

Each chapter is divided into numbered sections and subsections. Numbering of items like formulas, theorems and figures is done section-wise per chapter. Cross references to numbered items in other chapters are given explicitly with the chapter number in front.

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