Preface

In the analysis and the quest for an understanding of a physical system, generally, the formulation and use of a mathematical model that is thought to describe the system is an essential step. That is, a mathematical model is formulated (as a system of equations) that is thought to quantitatively define the interrelationships between phenomena that define the characteristics of the physical system. The mathematical model is usually tested against observations of the physical system, and if the agreement is considered acceptable, the model is then taken as a representation of the physical system, at least until improvements in the observations lead to refinements and extensions of the model. Often the model serves as a guide to new observations. Ideally, this process of refinement of the observations and model leads to improvements of the model and thus enhanced understanding of the physical system.

However, this process of comparing observations with a proposed model is not possible until the model equations are solved to give a solution that is then the basis for the comparison with observations. The solution of the model equations is often a challenge. Typically in science and engineering this involves the integration of systems of ordinary and partial differential equations (ODE/PDEs). The intent of this volume is to assist scientists and engineers in the process of solving differential equation models by explaining some numerical, computer-based methods that have generally been proved to be effective for the solution of a spectrum of ODE/PDE system problems.

For PDE models, we have focused on the method of lines (MOL), a well-established numerical procedure in which the PDE spatial (boundary-value) partial derivatives are approximated algebraically, in our case, by finite differences (FDs). The resulting differential equations have only one independent variable remaining, an initial-value variable, typically time in a physical application. Thus, the MOL approximation replaces a PDE system with an initial-value ODE system. This ODE system is then integrated using a standard routine, which, for the Matlab analysis used in the example applications, is one of the Matlab library integrators. In this way, we can take advantage of the recent progress in ODE numerical integrators.

However, while we have presented our MOL solutions in terms of Matlab code, it is not our intention to provide optimized Matlab code but, rather, to provide code that will be readily understood and that can be easily converted to other computer languages. This approach has been adopted in view of our experience that there is considerable interest in numerical solutions written in other computer languages such as Fortran, C, C++, and Java. Nevertheless, discussion of specific Matlab proprietary routines is included where this is thought to be of benefit to the reader.

Important variations on the MOL are possible. For example, the PDE spatial derivatives can be approximated by finite elements, finite volumes, weighted residual methods, and spectral methods. All of these approaches have been used and are described in the numerical analysis literature. For our purposes, and to keep the discussion to a reasonable length, we have focused on FDs. Specifically, we provide library routines for FDs of orders 2–10.

Our approach to describing the numerical methods is by example. Each chapter has a common format consisting of:

- An initial statement of the concepts in mathematics and computation discussed in the chapter.
- A statement of the equations to be solved numerically. These equations are a mathematical model that can originate from the analysis of a physical system. However, we have broadened the usual definition of a mathematical model for a physical system to also include equations that test a numerical method or algorithm, and in this sense, they are a model for the algorithm.

  Parenthetically, the selected PDE applications include some of the classical (we might even say "famous") PDEs. For example, we discuss the Euler and Navier Stokes equations of fluid dynamics with the Burgers equation as a special case, the Maxwell equations of electromagnetic field theory with the wave equation as a special case, and the Korteweg–deVries equation to illustrate some basic properties of solitons (as illustrated on the cover). The versatility of the MOL analysis is illustrated by linear and nonlinear PDEs in one dimension (1D), 2D, and 3D with a variety of boundary conditions, for example, Dirichlet, Neumann, and third type.
- A listing of a complete, commented computer program or code, written in Matlab, to solve the model equations. Thus, the programming is all in one place, and therefore a back-and-forth study of the chapter and programming located elsewhere (e.g., on a CD or in a Web link) is not required (although all of the Matlab routines are available from the Web site http://www.pdecomp.net).
- A step-by-step explanation of the code, with emphasis on the associated mathematics and computational algorithms at each step.
- A discussion of the output from the code, both numerically tabulated and plotted. In particular, the details of the solution that demonstrate features of the model equations and characteristics of the numerical algorithm are highlighted. The graphical output is typically in 2D and 3D, and in some applications includes movies/animations.
- The output is also evaluated with respect to accuracy, either by comparison with an analytical (exact) solution when available or by inference from changes in the approximations used in the numerical algorithms.
- A summary at the end of the chapter to reiterate (a) the general features and limitations of the numerical algorithm, and (b) the class of problems that the numerical algorithm can address.

All of the models in this volume are based on PDEs. However, because of the use of the MOL (again, in which the PDEs are replaced by systems of approximating ODEs), both ODEs and PDEs are covered along with associated algorithms. Our expectation is that the different types of models, covering all of the major classes of PDEs (parabolic, hyperbolic, elliptic), will provide a starting point for the numerical study of the ODE/PDE system of interest. This might be a straightforward modification of a computer code or extend to the development of a new code based on the ideas presented in one or more examples.

To this end, the chapters are essentially self-contained; they do not require reading the preceding chapters. Rather, we have tried to explain all of the relevant ideas within each chapter, which in some instances requires some repetition between chapters. Also, other chapters are occasionally mentioned for additional details, but it is not necessary to read those chapters. Six appendices are also included to cover concepts that are relevant to more than a single chapter.

We hope this format of self-contained chapters, rather than a chapter-to-chapter format, will be helpful in minimizing the reading and studying required to start the solution to the ODE/PDE system of interest. We welcome your comments about this organization, and your questions about any of the concepts and details presented, as reflected in the following lists of topics. We think these lists, along with the table of contents and the concluding index, will point to the chapters and pages relevant to the problem of interest.

Topic	**Chapter**
Burgers equation	5
Characteristics of hyperbolic PDEs	8
Complex PDEs	6
Conservation principles	13
Continuation methods	11
Coordinate-free operators	5, 9, 14
Cylindrical coordinates	13
Cubic Schrodinger equation	6
D'Alembert solution	8
Differential-algebraic equations (DAEs)	12
Differential operators	5, 9
Dirichlet boundary conditions	2, 5, 11
Discontinuous solutions	5, 8
Euler equations	5
Exact (analytical) solutions	1, 2, 3, 4, 5, 6, 7, 8, 10, 11, 12
Finite-difference library routines	1, 2, 3, 5, 9, 14
Finite differences (FDs)	1, 2
Front sharpening	5
Green's function analysis	3
h- and p-refinement	5, 9, 11
Helmholtz's equation	10
Higher-order FDs	1, 4
Implicit ODEs	12
Infinite spatial domains	6, 7, 8

Topic	Chapter
Inhomogeneous PDEs	4, 11
Integral invariants	3, 7
Jacobian matrix	7, 9
Korteweg–deVries equation	7
Laplace's equation	10, 11
Linear PDEs	2
Maxwell's equations	9
Method of lines (MOL)	1
Mixed boundary conditions	11, 13
Mixed (hyperbolic–parabolic) PDEs	9, 13
Mixed partial derivatives	12
Navier Stokes equations	5
Neumann boundary conditions	2, 5, 11, 13, 14
Nonlinear PDEs	4, 5, 6, 7, 13
Numerical quadrature	3, 7
Numerical solution accuracy	1, 2, 3, 4, 5, 6, 7, 8, 10, 11, 12
PDE derivations	5, 13
PDE simplification	5, 9
PDE test problems	9
Poisson's equation	10
Robin boundary conditions	11, 13
Second-order PDEs	8, 9
Shock formation	5
Simultaneous PDEs	4, 6, 13
Singularities	13, 14
Solitons	7
Source terms	11, 13, 14
Sparse matrix integration	6, 7, 9
Spatial convergence	5, 9
Spherical coordinates	14
Stagewise differentiation	3, 5, 12
Tensors	5
Third-type boundary conditions	11, 13
Three-dimensional PDEs	11
Traveling wave solutions	5, 6, 7, 8
Two-dimensional PDEs	10, 13, 14
Units in PDEs	13
Variable-coefficient PDEs	4, 13, 14
Vector operators	5, 9
Wave equation	8, 9

This list contains primarily mathematical topics. The programming in each of the chapters is also a major topic.

The six appendices cover the following topics:

Topic	Appendix
Algebraic grid points	4
Analytical solutions	3
Anisotropic diffusion	1
Cartesian coordinates	1
Conservation principles	1
Cylindrical coordinates	1
Differential grid points	4
Differential operators	1
Dirichlet boundary conditions	4
Finite-difference order conditions	2
Finite-difference test problems	2
Finite differences (FDs)	2, 5
Library FD routines	5
Movies/animations	6
PDE derivations	1
Spherical coordinates	1
Tensors	1
Time-varying boundary conditions	4
Traveling waves	3
Truncation error	2
Vector operators	1

We have assumed a background of basic calculus and ODEs. Since the central algorithm is the MOL, we begin with a MOL introduction in Chapter 1. Then the chapters progress through example applications of increasing complexity and diversity. The preceding list serves as a guide for specific topics.

We have not included exercises at the end of the chapters since we think variations in the applications and the associated Matlab codes provide ample opportunities for exploration and further study. References are provided at the end of the chapters and appendices when we think they would provide useful additional background, but we have not attempted a comprehensive list of references on any particular topic.

Our intent for this volume is to present mathematical and computational methods that can be applied to a broad spectrum of ODE/PDE models. In particular, we are attempting to assist engineers and scientists who have an ODE/PDE problem of interest and who wish to produce an accurate numerical solution with reasonable computational effort without having to first delve into the myriad details of numerical methods and computer programming. We hope this book is of assistance toward meeting this objective.

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