Partial Differential Equation Analysis in Biomedical Engineering

Case Studies with MATLAB

Aimed at graduates and researchers, and requiring only a basic knowledge of multivariable calculus, this introduction to computer-based partial differential equation (PDE) modeling provides readers with the practical methods necessary to develop and use PDE mathematical models in biomedical engineering. Taking an applied approach, rather than using abstract mathematics, the reader is instructed through six biomedical example applications, each example characterized by step-by-step discussions of established numerical methods, and implemented in reliable computer routines. Adopting this technique, the reader will understand how PDE models are formulated, implemented and tested. Supported by a set of rigorously tested general purpose PDE routines online, and with enhanced understanding through animations, this book will be ideal for anyone faced with interpreting large experimental data sets that need to be analyzed with PDE models in biomedical engineering.

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To my parents
Laura Virginia Bauer
Edward Valentine Schiesser

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Preface

This book is an introduction to the mathematical modeling of biomedical engineering systems. In particular, models based on partial differential equations (PDEs) are presented: antibody binding kinetics, acid-mediated tumor growth, retinal O_2 transport, hemodialyzer dynamics, epidermal wound healing, and polymer matrix drug delivery.

The numerical solution of the model equations is through a single, well-established method for PDEs, the method of lines (MOL), in which the spatial derivatives in the PDEs are replaced with algebraic approximations and a system of ordinary differential equations (ODEs) in an initial value variable, typically time, follows. The spatial approximations are finite differences (FDs), although other approximations could easily be accommodated within the MOL format, e.g., finite elements, finite volumes, spectral methods, Galerkin methods such as collocation, meshfree methods. The final result is a set of routines that numerically integrates the ODEs; the format of these routines is basically the same throughout the book.

To facilitate understanding of the PDE analysis, an introduction to the numerical methods and associated computational routines is presented in the first chapter. Then each application is cross referenced to this introduction in each step where some additional explanation is helpful.

In each example, we follow a combination of the following steps:

- Statement of the model PDE, along with the associated auxiliary (initial and boundary) conditions. This introduction to the model contains a reference to the original source and possibly related literature, and includes some discussion of the underlying biophysics, biochemistry, and physiology.
- Discussion of the numerical methods (algorithms) for the MOL solution of the model equations, principally by reference to the introduction in Chapter 1.
- List of MATLAB routines based on the MOL numerical solution of the PDEs, discussed in some detail, typically a few lines of code at a time. This discussion emphasizes how the associated mathematics of the model is programmed.
- Discussion of the numerical solution of the model equations, including the origin of any unusual features of the solution.
- Error analysis to establish if the numerical solution is reliable and has acceptable accuracy; typically techniques such as varying the MOL grid spacing and order of approximation are used to infer convergence of the numerical solution to an acceptable

level of accuracy. Also, physical constraints such as conservation of mass energy and energy are used to evaluate the solution.

- Concluding summary and discussion of extensions of the model and the MOL algorithms.

Our intention is not to provide a comprehensive treatise, but rather to provide a set of basic computational procedures that we hope readers can assimilate without becoming deeply involved in the details of numerical methods for PDEs and computer programming so that they can concentrate on the problem of interest with reasonable effort. This might take the form of extending the computer routines provided, or applying and extending the numerical methods that are presented through examples.

In summary, our intention is to provide a methodology for the PDE analysis of biomedical engineering systems. This includes the development of numerical methods and associated computer routines that can be used to study the characteristics and solutions of the model equations. The approach is not theoretical, e.g., limited theorems and no proofs; rather, the presentation is based on detailed example applications. The MOL analysis provides a general framework for the analysis of PDE models that we think can be broadly applied in biomedical engineering, and which can be applied to all of the major geometric classes of PDEs (parabolic, hyperbolic, elliptic). All of the MATLAB routines are available (gratis) as a download through a request to wes1@lehigh.edu.

We welcome comments from readers concerning this approach and will be pleased to answer questions to the extent possible by e-mail.