TEXTBOOKS in MATHEMATICS

COMPUTATIONAL MATHEMATICS

Models, Methods, and Analysis with MATLAB® and MPI

Second Edition

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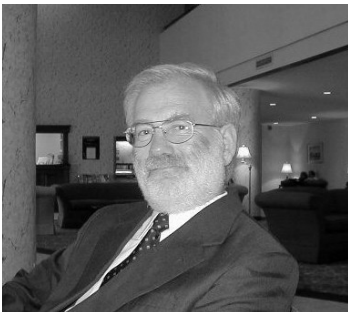
Preface to First Edition

This book evolved from the need to migrate computational science into undergraduate education. It is intended for students who have had basic physics, programming, matrices, and multivariable calculus.

The choice of topics in the book has been influenced by the Undergraduate Computational Engineering and Science Project (a United States Department of Energy funded effort), which was a series of meetings during the 1990s. These meetings focused on the nature and content for computational science undergraduate education. They were attended by a diverse group of science and engineering teachers and professionals, and the continuation of some of these activities can be found at the Krell Institute, http://www.krellinst.org. Variations of Chapters 1–4 and 6 have been taught at North Carolina State University in fall semesters since 1992. The other four chapters were developed in 2002 and taught in the 2002–03 academic year.

The department of mathematics at North Carolina State University has given me the time to focus on the challenge of introducing computational science materials into the undergraduate curriculum. The North Carolina Supercomputing Center, http://www.ncsc.org, has provided the students with valuable tutorials and computer time on supercomputers. Many students have made important suggestions, and Carol Cox Benzi contributed some course materials with the initial use of MATLAB®.

I thank my close friends who have listened to me talk about this effort, and especially Liz White who has endured the whole process with me.



Bob White, July 1, 2003

Preface to Second Edition

The second edition has a new Chapter 5 with two sections on the finite element method, two sections on shallow water waves, and two sections on the driven cavity problem. The old Chapter 5 is now Chapter 6 with the same applications to population models, image restoration, and option contracts. The old Chapter 6 is the new Chapter 7, and it has been reorganized to include introductions to multiprocessor/multicore computers, parallel MATLAB®, and MPI. Chapters 1 to 4 have formed the core of an undergraduate course with an emphasis on numerical models evolving from partial differential equations. A second course on an introduction to high-performance computing has more graduate students, and its core is from Chapters 7 to 10. Chapters 5 and 6 are a little more terse and contain a selection of six applications. Sections 3.3, 3.4, and 5.3–5.6 form a nice introduction to computational fluids, and Sections 4.6, and 7.1–7.6 form an introduction to parallel programming.

Most of the MATLAB codes have been rewritten to have a more uniform style and with better documentation. Also, parallel MATLAB is introduced at the end of Chapter 4 and in Chapter 7. All the computer codes can be found at

http://www4.ncsu.edu/eos/users/w/white/www/book/filename

where *filename* is the name of the code file, for example, heat3d.m or trapmpi.f90 or trapmpisub or trapmpimake. A large number of codes has been included so as to give the student a "step-up" in learning computation and numerical modeling for partial differential equations.

In the exercises there are six "projects," which are usually done by groups of two or three students. The first four projects are associated with Chapters 1 to 4 (see the end of Sections 1.5, 2.3, 3.2, and 3.4). The last two projects are associated with Chapters 7 and 9 (see the end of Sections 7.6 and 9.3). The six applications in Chapters 5 and 6 could also form a basis for additional projects. Many of the graduate students have active projects in their major field of study, and here it has been beneficial to include student–instructor defined projects.

This text is an introduction to models that are nonlinear, 2D and 3D, nonrectangular domains, systems of PDEs, and large algebraic problems that require high-performance computing. The emphasis is more modeling and computation and less analysis. Although it does not replace traditional numerical analysis, linear algebra, and partial differential equation courses, topics from these courses are developed as needed in parts of Sections 1.1, 1.6, 2.1–2.6, 3.1, 3.5, 4.1, 9.1, 9.2, 9.4, 10.1, 10.4, and 10.5.

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Introduction

Computational science is a blend of applications, computations, and mathematics. It is a mode of scientific investigation that supplements the traditional laboratory and theoretical methods for acquiring knowledge. This is done by formulating mathematical models whose solutions are approximated by computer simulations. By making a sequence of adjustments to the model and subsequent computations one can gain some insights into the application area under consideration. This text attempts to illustrate this process as a method for scientific investigation. Each section of the first six chapters is motivated by a particular application, discrete or continuous model, numerical method, computer implementation, and an assessment of what has been done.

Applications include heat diffusion to cooling fins and solar energy storage, pollutant transfer in streams and lakes, models of vector and multiprocessing computers, ideal and porous fluid flows, deformed membranes, shallow water waves, fluid flow in a cavity, epidemic models with dispersion, image restoration, and the value of American put option contracts. The models are initially introduced as discrete in time and space, and this allows for an early introduction to partial differential equations. The discrete models have the form of matrix products or linear and nonlinear systems. Methods include sparse matrix iteration with stability constraints, sparse matrix solutions via variation on Gauss elimination, successive over-relaxation, conjugate gradient, and minimum residual methods. Picard and Newton methods are used to approximate the solution to nonlinear systems.

Most sections in the first six chapters have MATLAB® codes; see [19] for the very affordable current student version of MATLAB. They are intended to be studied and not used as a "black box." The MATLAB codes should be used as a first step toward more sophisticated numerical modeling. These codes do provide a learning-by-doing environment. The exercises at the end of each section have three categories: routine computations, variation of models, and mathematical analysis. The last four chapters focus on multiprocessing algorithms, which are implemented using message passing interface, MPI. These chapters have elementary Fortran 9x codes to illustrate the basic MPI subroutines, and the applications of the previous chapters are revisited from a parallel implementation perspective.

This text is not meant to replace traditional texts on numerical analysis, matrix algebra, and partial differential equations. It does develop topics in these areas as is needed and also includes modeling and computation, and so there is more breadth and less depth in these topics. One important component of computational science is parameter identification and model validation, and this requires a physical laboratory to take data from experiments. In this text model assessments have been restricted to the variation of model parameters, model evolution, and mathematical analysis. More penetrating expertise in various aspects of computational science should be acquired in subsequent courses and work experiences.

Related computational mathematics education material at the first-year and second-year undergraduate level can be found at the Shodor Education Foundation, whose founder is Robert M. Panoff, website [28] and in Zachary's book on programming [38]. Two general references for modeling are the undergraduate mathematics journal [33] and Beltrami's book on modeling for society and biology [4]. Both of these have a variety of models, but often there are no computer implementations, so they are a good source of potential computing projects. The book by Landau and Paez [17] has a number of computational physics models, which are at about the same level as this book. Slightly more advanced numerical analysis references are by Fosdick, Jessup, Schauble and Domik [10], Heath [14], and Strang[31].

The computer codes and updates for this book can be found at the website

http://www4.ncsu.edu/˜white.

The computer codes are mostly in MATLAB for the first six chapters, and in Fortran 9x for most of the MPI codes in the last four chapters. The choice of Fortran 9x is the author's personal preference as the array operations are similar to those in MATLAB. However, the above website and the website associated with Pacheco's book [26] do have C versions of these and related MPI codes.