Computational Mathematics: Models, Methods and Analysis *with* MATLAB and MPI

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Preface

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®. MATLAB is a registered trademark of The MathWorks, Inc. For product information, please contact:

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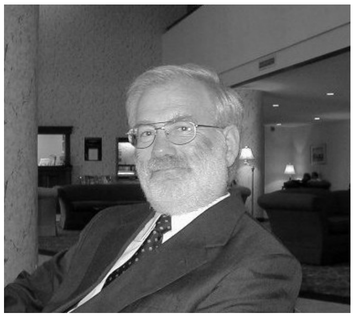
I thank my close friends who have listened to me talk about this effort, and especially Liz White who has endured the whole process with me.



Bob White, July 1, 2003

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 of 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, epidemic models with dispersion, image restoration and 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 five chapters have MATLAB® codes; see [14] 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 towards 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; see [17] for information about building your own multiprocessor via free "NPACI Rocks" cluster software. 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.

At North Carolina State University Chapters 1-4 are covered in 26 75-minute lectures. Routine homework problems are assigned, and two projects are required, which can be chosen from topics in Chapters 1-5, related courses or work experiences. This forms a semester course on numerical modeling using partial differential equations. Chapter 6 on high performance computing can be studied after Chapter 1 so as to enable the student, early in the semester, to become familiar with a high performance computing environment. Other course possibilities include: a semester course with an emphasis on mathematical analysis using Chapters 1-3, 8 and 9, a semester course with a focus on parallel computation using Chapters 1 and 6-9 or a year course using Chapters 1-9.

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 and second year undergraduate level can be found at the Shodor Education Foundation, whose founder is Robert M. Panoff, web site [22] and in Zachary's book on programming [29]. Two general references for modeling are the undergraduate mathematics journal [25] and Beltrami's book on modeling for society and biology [2]. Both of these have a variety of models, but often there are no computer implemenations. So they are a good source of potential computing projects. The book by Landau and Paez [13] has 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 [7] and Heath [10].

The computer codes and updates for this book can be found at the web site:

http://www4.ncsu.edu/~white.

The computer codes are mostly in MATLAB for Chapters 1-5, and in Fortran 9x for most of the MPI codes in Chapters 6-9. The choice of Fortran 9x is the author's personal preference as the array operations are similar to those in MATLAB. However, the above web site and the web site associated with Pacheco's book [21] do have C versions of these and related MPI codes. The web site for this book is expected to evolve and also has links to sequences of heat and pollution transfer images, book updates and new reference materials.