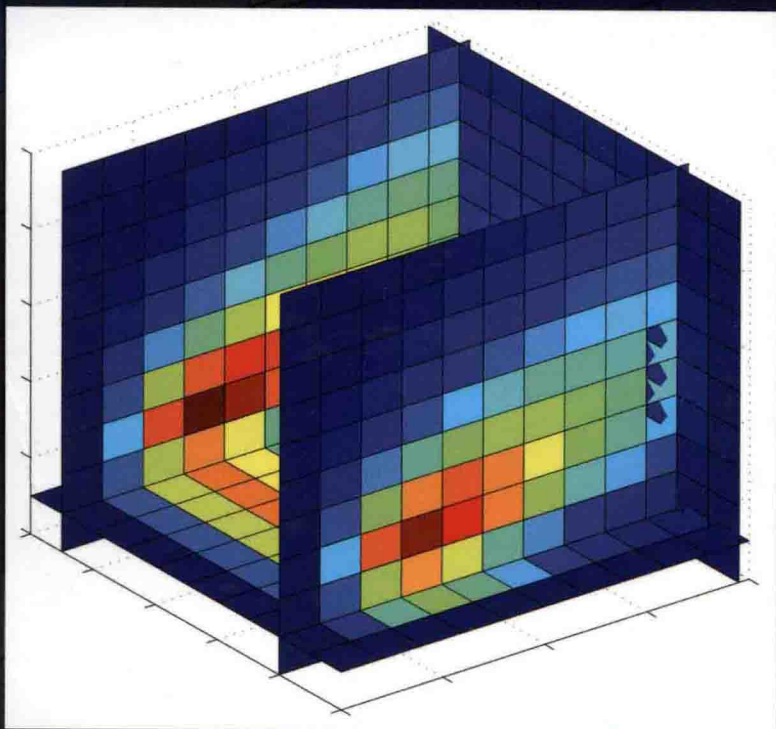


TEXTBOOKS in MATHEMATICS

# COMPUTATIONAL MATHEMATICS

Models, Methods, and Analysis  
with MATLAB® and MPI

Second Edition



Robert E. White



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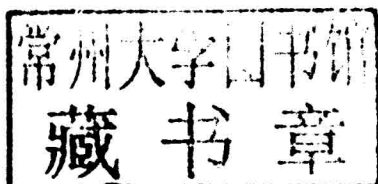
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ROBERT E. WHITE

North Carolina State University  
Raleigh, North Carolina, USA



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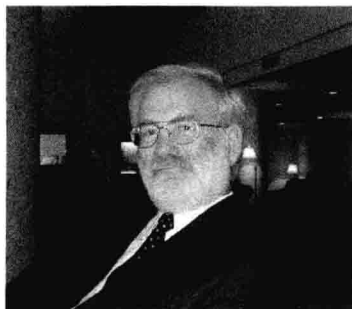
# Preface to First Edition

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<sup>®</sup>.

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<sup>®</sup>, 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, non-rectangular 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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