

TEXTBOOKS in MATHEMATICS

COMPUTATIONAL MATHEMATICS

Models, Methods, and Analysis
with MATLAB[®] and MPI
Second Edition

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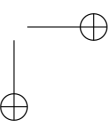
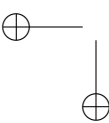
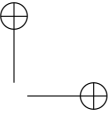
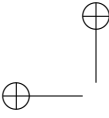
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Contents

List of Figures	xi
List of Tables	xv
Preface to First Edition	xvii
Preface to Second Edition	xix
Introduction	xxi
1 Discrete Time–Space Models	1
1.1 Newton Cooling Models	1
1.2 Heat Diffusion in a Wire	9
1.3 Diffusion in a Wire with Little Insulation	18
1.4 Flow and Decay of a Pollutant in a Stream	26
1.5 Heat and Mass Transfer in Two Directions	34
1.6 Convergence Analysis	45
2 Steady-State Discrete Models	55
2.1 Steady-State and Triangular Solves	55
2.2 Heat Diffusion and Gauss Elimination	63
2.3 Cooling Fin and Tridiagonal Matrices	74
2.4 Schur Complement	83
2.5 Convergence to Steady-State Solution	92
2.6 Convergence to Continuous Model	99
3 Poisson Equation Models	107
3.1 Steady-State and Iterative Methods	107
3.2 Heat Transfer in 2D Fin and SOR	117
3.3 Fluid Flow in a 2D Porous Medium	125
3.4 Ideal Fluid Flow	132
3.5 Deformed Membrane and Steepest Descent	141
3.6 Conjugate Gradient Method	150

4	Nonlinear and 3D Models	161
4.1	Nonlinear Problems in One Variable	161
4.2	Nonlinear Heat Transfer in a Wire	169
4.3	Nonlinear Heat Transfer in 2D	177
4.4	Steady-State 3D Heat Diffusion	183
4.5	Time-Dependent 3D Diffusion	189
4.6	High-Performance Computations in 3D	197
5	FEM and Fluid Flows	209
5.1	FEM and Linear Shape Functions	209
5.2	FEM with Heat and Fluid Flow	218
5.3	Lax-Wendroff Methods	226
5.4	Shallow Water Wave Model	232
5.5	Navier-Stokes Equations	237
5.6	Discrete Navier-Stokes Equations	240
6	Epidemics, Images, and Money	247
6.1	Epidemics and Dispersion	247
6.2	Epidemic Dispersion in 2D	255
6.3	Image Restoration	262
6.4	Restoration in 2D	271
6.5	Option Contract Models	277
6.6	Black-Scholes Model for Two Assets	286
7	High-Performance Computing	295
7.1	CPUs and Vector Pipes	295
7.2	Multiprocessor and Multicore Computers	307
7.3	Parallel MATLAB [®]	316
7.4	Parallel MATLAB and SPMD	326
7.5	Introduction to MPI	334
7.6	MPI and Matrix Products	343
8	Message Passing Interface	355
8.1	Collective Subroutines	355
8.2	Grouped Datatypes	367
8.3	Communicators	374
8.4	Fox Algorithm for AB	380
8.5	Shared Memory and OpenMP	386
8.6	Hybrid MPI/OpenMP	392
9	Classical Methods for $Ax = d$	399
9.1	Gauss Elimination	399
9.2	Symmetric Positive Definite Matrices	404
9.3	Domain Decomposition and MPI	410
9.4	SOR and P-Regular Splittings	415
9.5	SOR and MPI	420

<i>CONTENTS</i>	ix
9.6 Parallel ADI Schemes	426
10 Krylov Methods for $Ax = d$	431
10.1 Conjugate Gradient Method	431
10.2 Preconditioners	436
10.3 PCG and MPI	442
10.4 Least Squares	446
10.5 GMRES	453
10.6 GMRES(m) and MPI	460
Bibliography	467
Index	471



List of Figures

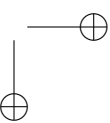
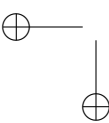
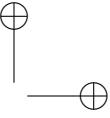
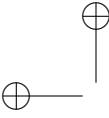
1.1.1 Temperature versus time.	6
1.1.2 Steady-state temperature.	7
1.1.3 Unstable computation.	7
1.2.1 Diffusion in a wire.	11
1.2.2 Time–space grid.	13
1.2.3 Temperature versus time–space.	15
1.2.4 Unstable computation.	16
1.2.5 Steady-state temperature.	16
1.3.1 Diffusion in a wire with $csur = 0.0000$ and 0.0005	23
1.3.2 Diffusion in a wire with $n = 5$ and 20	24
1.4.1 Polluted stream.	27
1.4.2 Concentration of pollutant.	31
1.4.3 Unstable concentration computation.	33
1.5.1 Heat or mass entering or leaving.	36
1.5.2 Temperature at final time.	39
1.5.3 Heat diffusing out a fin.	40
1.5.4 Concentration at the final time.	42
1.5.5 Concentrations at different times.	43
1.6.1 Euler approximations.	48
2.1.1 Infinite or none or one solution(s).	56
2.2.1 Gaussian elimination.	69
2.3.1 Thin cooling fin.	75
2.3.2 Temperatures for $c = 0.1, 0.01, 0.001,$ and 0.0001	81
2.6.1 Variable $r = 0.1, 0.2,$ and 0.3	102
2.6.2 Variable $n = 4, 8,$ and 16	103
3.1.1 Cooling fin with $T = 0.05, 0.10,$ and 0.15	114
3.2.1 Diffusion in two directions.	117
3.2.2 Temperatures and contours of fin.	122
3.2.3 Cooling fin grid.	123
3.3.1 Incompressible 2D fluid.	126
3.3.2 Groundwater 2D porous flow.	127
3.3.3 Pressure for two wells.	132

3.4.1	Ideal flow about an obstacle.	133
3.4.2	Irrotational 2D flow $v_x - u_y = 0$	134
3.4.3	Flow around an obstacle.	138
3.4.4	Two paths to (x,y)	139
3.5.1	Steepest descent norm(r).	148
3.6.1	Convergence for CG and PCG.	158
4.2.1	Change in F_1	171
4.2.2	Temperatures for variable C.	175
4.4.1	Heat diffusion in 3D.	184
4.4.2	Temperatures inside a 3D fin.	188
4.5.1	Passive solar storage.	190
4.5.2	Slab is gaining heat.	196
4.5.3	Slab is cooling.	196
4.6.1	Domain decomposition in 3D.	201
4.6.2	Domain decomposition matrix.	206
4.6.3	Electric potential.	207
5.1.1	Linear shape test function.	211
5.1.2	Triangular elements.	213
5.1.3	Test problem elements.	215
5.1.4	Triangular elements for the membrane.	217
5.1.5	Deformed membrane.	217
5.2.1	Heat transfer about a steam pipe.	224
5.2.2	Heat transfer in cooling fin for pipe.	224
5.2.3	Ideal flow about an obstacle.	225
5.3.1	Lax–Wendroff and two initial conditions.	228
5.3.2	Upwind and two initial conditions.	229
5.3.3	Velocity at different times.	230
5.4.1	Reflective boundary conditions.	233
5.4.2	Changing mass of a column.	235
5.4.3	Shallow water waves.	236
5.5.1	Driven flow in a cavity.	237
5.6.1	Staggered grid.	241
5.6.2	Driven cavity.	243
6.1.1	Infected and susceptible versus space.	254
6.2.1	Grid with artificial grid points.	257
6.2.2	Infected and susceptible at time = 0.3.	261
6.3.1	Three curves with jumps.	264
6.3.2	Restored 1D image.	270
6.4.1	Restored 2D image.	277
6.5.1	Value of American put option.	280
6.5.2	$P(S,T-t)$ for variable times.	284
6.5.3	Option values for variable volatilities.	284
6.5.4	Optimal exercise of an American put.	285

LIST OF FIGURES

xiii

6.6.1 American put with two assets.	287
6.6.2 $\max(E_1 + E_2 - S_1 - S_2, 0)$	292
6.6.3 $\max(E_1 - S_1, 0) + \max(E_2 - S_2, 0)$	292
7.1.1 von Neumann computer.	296
7.1.2 Shared memory multiprocessor.	297
7.1.3 Floating point add.	297
7.1.4 Bit adder.	297
7.1.5 Vector pipeline for floating point add.	299
7.1.6 Temperature in fin at $t = 60$	305
7.2.1 Ring and complete multiprocessors.	308
7.2.2 Hypercube multiprocessor.	308
7.2.3 Two-core chip with hyper-threading.	312
7.3.1 Divide-and-conquer data flow.	317
7.3.2 Fan-in data flow.	318
7.3.3 Domain-decomposition data flow.	319
7.4.1 Data flow for Newton method.	328
7.4.2 Data flow for explicit method.	330
7.4.3 Concentration at $t = 17$	334
7.5.1 Fan-out data flow.	342
7.6.1 Space grid with four subblocks.	349
7.6.2 Send and receive for processors.	350
8.4.1 Data flow for Fox method.	382



List of Tables

1.6.1 Euler Errors at $t = 10$	49
1.6.2 Errors for Flow	51
1.6.3 Errors for Heat	52
2.6.1 Second-Order Convergence	105
3.1.1 Variable SOR Parameter	114
3.2.1 Convergence and SOR Parameter	122
4.1.1 Quadratic Convergence	165
4.1.2 Local Convergence	165
4.2.1 Newton’s Rapid Convergence	175
4.6.1 Parallel Computing Times	206
5.3.1 Errors for 1D Flow	227
7.1.1 Truth Table for Bit Adder	298
7.1.2 Matrix–Vector Computation Times	301
7.1.3 Heat Diffusion Vector Times	302
7.2.1 Speedup and Efficiency	310
7.2.2 HPF for 2D Diffusion	311
7.3.1 Times for Sums	320
7.3.2 Times for Ax	322
7.3.3 Times for BC	324
7.5.1 MPI Times for trapempi.f	343
7.6.1 Matrix–Vector Product mflops	346
7.6.2 Matrix–Matrix Product mflops	348
7.6.3 Processor Times for Diffusion	352
8.4.1 Fox mflops	385
8.5.1 MPI Times for matvecomp.f90	391
8.6.1 MPI Times for trapmpiomp.f90	395
8.6.2 MPI Times for matvecmpiomp.f90	396
8.6.3 MPI Times for mmmmpiomp.f90	398

9.3.1 MPI Times for gedddmpi.f90	414
9.5.1 MPI Times for sorddmpi.f90	425
10.3. MPI Times for cgssormpi.f90	446
10.6. MPI Times for gmresmpi.f90	465

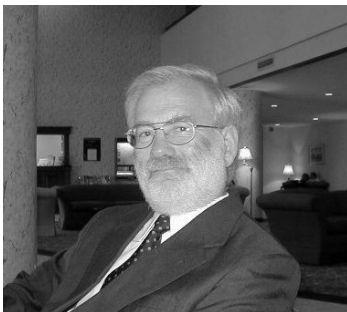
Preface to First Edition

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.

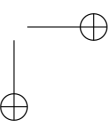
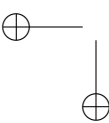
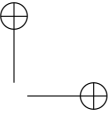
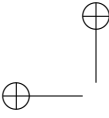
The choice of topics in the book has been influenced by the Undergraduate Computational Engineering and Science Project (a United States Department of Energy funded effort), which was a series of meetings during the 1990s. These meetings focused on the nature and content for computational science undergraduate 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, 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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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.