

Bertil Gustafsson

Fundamentals of Scientific Computing

 Springer

Bertil Gustafsson
Information Technology
Uppsala University
PO Box 337
751 05 Uppsala
Sweden
bertil.gustafsson@it.uu.se

ISSN 1611-0994
ISBN 978-3-642-19494-8 e-ISBN 978-3-642-19495-5
DOI 10.1007/978-3-642-19495-5
Springer Heidelberg Dordrecht London New York

Library of Congress Control Number: 2011929632

Mathematics Subject Classification (2000): 65-01

© Springer-Verlag Berlin Heidelberg 2011

This work is subject to copyright. All rights are reserved, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilm or in any other way, and storage in data banks. Duplication of this publication or parts thereof is permitted only under the provisions of the German Copyright Law of September 9, 1965, in its current version, and permission for use must always be obtained from Springer. Violations are liable to prosecution under the German Copyright Law.

The use of general descriptive names, registered names, trademarks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

Cover design: deblik, Berlin

Printed on acid-free paper

Springer is part of Springer Science+Business Media (www.springer.com)

Contents

Part I Models and Elementary Mathematics

1	Introduction	3
1.1	Computational Example 1	3
1.2	Computational Example 2	12
1.3	Outline of the Book	15
2	Mathematical Models	19
2.1	*Basic Concepts	19
2.2	*Ordinary Differential Equations	23
2.2.1	Derivatives	23
2.2.2	Differential Equations and Initial Value Problems	27
2.2.3	Integrals	30
2.2.4	More on Differential Equations and Discretization	32
2.3	**Partial Differential Equations	36
2.3.1	Partial Derivatives	36
2.3.2	Boundary and Initial-Boundary Value Problems	41
2.4	**Well Posed Mathematical Models	43
3	Basic Linear Algebra	47
3.1	*Vector Spaces	47
3.2	*Complex Numbers	52
3.3	*Matrix Algebra	54
3.4	**Eigenvalues	62
4	Analysis Tools	67
4.1	*Infinite Processes	67
4.1.1	Infinite Number Sequences	68
4.1.2	Infinite Series	69
4.2	*Taylor Series	72
5	Elementary Functions	77
5.1	*Polynomials	77

- 5.1.1 Standard Polynomials 77
- 5.1.2 Piecewise Polynomials 83
- 5.1.3 Orthogonal Polynomials 89
- 5.2 *Trigonometric Functions 90
- 5.3 **The Exponential Function 93

Part II Fundamentals in Numerical Analysis

- 6 The Fourier Transform 103**
 - 6.1 Fourier Series 104
 - 6.2 The Discrete Fourier Transform 109
- 7 Polynomial Expansions 117**
 - 7.1 Orthogonal Polynomial Expansions 117
 - 7.2 Chebyshev Polynomials 118
 - 7.3 Legendre Polynomials 122
- 8 Least Square Problems 125**
 - 8.1 Vector Approximations 125
 - 8.2 The Continuous Case 127
 - 8.3 The Discrete Case 129

Part III Numerical Methods for Differential Equations

- 9 Numerical Methods for Differential Equations 137**
 - 9.1 Basic Principles 137
 - 9.2 Resolution 142
- 10 Finite Difference Methods 145**
 - 10.1 Ordinary Differential Equations 145
 - 10.2 Partial Differential Equations 158
 - 10.3 Fourier Stability Analysis 162
 - 10.4 Several Space Dimensions 167
- 11 Finite Element Methods 173**
 - 11.1 Boundary Value Problems 173
 - 11.2 Initial-Boundary Value Problems 184
 - 11.3 Discontinuous Galerkin Methods 186
- 12 Spectral Methods 193**
 - 12.1 An Example with a Sine Expansion 193
 - 12.2 Fourier Methods 198
 - 12.3 Polynomial Methods 201

Part IV Numerical Methods for Algebraic Equations

- 13 Numerical Solution of Nonlinear Equations 205**
 - 13.1 Scalar Nonlinear Equations 205
 - 13.2 Vector Equations 209

14 Linear Systems of Equations 213

14.1 The Condition of a System 213

14.2 Direct Methods 215

14.3 Iterative Methods 218

14.4 Preconditioning 227

14.5 Multigrid Methods 227

Part V Applications

15 Wave Propagation 235

15.1 Hyperbolic PDE 235

15.2 Acoustics 240

15.3 Electromagnetics 246

15.4 Other Types of Wave Propagation 252

15.4.1 Elasticity 252

15.4.2 The Schrödinger Equation 253

16 Heat Conduction 255

16.1 Parabolic PDE 255

16.2 Elliptic PDE 258

16.3 The Heat Equation 259

17 Fluid Dynamics 263

17.1 Basic Differential Equations 263

17.1.1 The Continuity Equation 264

17.1.2 Euler equations 265

17.1.3 Shocks 267

17.1.4 Incompressible Navier–Stokes Equations 270

17.2 Low Speed Flow 277

17.3 High Speed Flow and Aircraft Design 280

17.4 Weather Prediction 285

18 Computers and Programming 291

18.1 Basic Principles for Programming 291

18.2 MATLAB 293

18.3 Parallel Computers 300

19 Further Reading 303

Erratum to: Basic Linear Algebra E1

Appendix Mathematical Rules 305

A.1 Rules for Differentiation 305

A.2 Differential Operators in Different Coordinate Systems 306

A.2.1 2D 306

A.2.2 3D 306

A.3 Trigonometric Formulas 307

A.4 Matrix Algebra 308

References 311

Index 313