

Contents

1	Scientific Modeling	1
1.1	Reality Versus Model	1
1.2	The Model Subject and the Model	3
1.2.1	The Purpose of a Model	3
1.3	The Model Subject and Reality	4
1.4	Model Building	5
1.4.1	Problem Specification	5
1.4.2	Creating a Structural Concept	5
1.4.3	Choosing and Designing a Model	6
1.4.4	Establishing Parameter Values	8
1.4.5	Tests and Validation	8
2	Fundamental Principles of Numerical Methods	9
2.1	From Application Problems to their Numerical Solution	9
2.1.1	Case Study: Pendulum	10
2.1.2	Qualitative and Quantitative Problems	14
2.2	Numerical Problems	16
2.2.1	Numerical Problems	19
2.2.2	Categories of Numerical Problems	21
2.2.3	The Accuracy of Numerical Results	23
2.3	Types of Errors in Numerics	28
2.3.1	Model Errors	29
2.3.2	Data Errors	29
2.3.3	Algorithm Errors	30
2.3.4	Rounding Errors	34
2.3.5	Error Hierarchy	37
2.4	The Condition of Mathematical Problems	39
2.4.1	Perturbed and Unperturbed Problems	39
2.4.2	The Absolute Condition Number	39
2.4.3	The Relative Condition Number	40
2.4.4	Narrowing the Problem Class	42
2.4.5	Calculating Condition Numbers Using Differentiation	42
2.4.6	Case Study: Quadratic Equation	43
2.4.7	Ill-Conditioned Problems	44
2.4.8	Ill-Posed Problems	45
2.5	The Condition of Application Problems	46
2.6	The Mathematical Elements of Condition Estimation	48
2.6.1	The Condition of Direct Mathematical Problems	48
2.6.2	The Condition of Inverse Mathematical Problems	54
2.7	Validation of Numerical Computations	58

2.7.1	The Uncertainty of Numerical Computations	58
2.7.2	Validation of Mathematical Models	59
2.7.3	Sensitivity Analysis and Error Estimation	60
2.7.4	Validation of Numerical Software	65
3	Computers for Numerical Data Processing	68
3.1	Processors	70
3.1.1	Pipelining	71
3.1.2	Superpipeline Architecture	75
3.1.3	Superscalar Architectures	75
3.1.4	Vector Processors	77
3.2	Memory	78
3.2.1	Memory Hierarchy	79
3.2.2	Addressing Schemes	81
3.2.3	Registers	82
3.2.4	Cache Memory	83
3.2.5	Virtual Memory	88
3.2.6	Interleaved Memory	89
3.3	Performance Quantification	90
3.3.1	The Notion of Performance (Power)	91
3.3.2	Time as a Factor in Performance	92
3.4	Analytical Performance Assessment	94
3.4.1	Peak Performance	94
3.4.2	Instruction Performance	95
3.4.3	Performance of Vector Processors	97
3.4.4	The Influence of Memory on Performance	100
3.5	Empirical Performance Assessment	101
3.5.1	Temporal Performance	101
3.5.2	Empirical Instruction Performance	101
3.5.3	Empirical Floating-Point Performance	102
3.5.4	Empirical Performance of Vector Processors	104
4	Numerical Data and Numerical Operations	106
4.1	Mathematical Data	106
4.1.1	Fundamental Mathematical Data	106
4.1.2	Algebraic Data	106
4.1.3	Analytic Data	107
4.2	Numerical Data on Computers	108
4.2.1	Fundamental Numerical Data	108
4.2.2	Algebraic Data	110
4.2.3	Analytic Data	110
4.2.4	Numerical Data Types	110
4.3	Operations on Numerical Data	111
4.3.1	Arithmetic Operations	111
4.3.2	Algebraic Operations	112

4.3.3	Array Processing in Fortran 90	113
4.3.4	Analytic Operations	116
4.4	Number Systems on Computers	117
4.4.1	INTEGER Number Systems	118
4.4.2	Fixed-Point Number Systems	120
4.4.3	Floating-Point Number Systems	122
4.5	Structure of Floating-Point Systems	126
4.5.1	The Number of Floating-Point Numbers	126
4.5.2	Largest and Smallest Floating-Point Numbers	127
4.5.3	Distances Between Floating-Point Numbers	128
4.5.4	Relative Distances Between Floating-Point Numbers	129
4.5.5	Case Study: $\mathbb{F}(10, 6, -9, 9, \text{true})$	131
4.6	Standardization of Floating-Point Number Systems	132
4.6.1	The IEEE Standard for Floating-Point Numbers	132
4.6.2	Hidden Bit	134
4.6.3	Infinity, NaNs, and Signed Zero	134
4.6.4	Impact on Programming Languages	134
4.7	Arithmetics for Floating-Point Systems	135
4.7.1	Rounding Functions	136
4.7.2	Rounding Error	139
4.7.3	Rounding and Arithmetic Operations	142
4.7.4	Implementation of a Floating-Point Arithmetic	146
4.7.5	Multiple-Precision Software	147
4.8	Inquiry Functions and Manipulation of Numbers in Fortran 90	151
4.8.1	Parameters for Floating-Point Numbers	151
4.8.2	Characteristics of Floating-Point Numbers	152
4.8.3	The Distance Between Floating-Point Numbers, Rounding	154
4.8.4	Manipulation of Floating-Point Numbers	155
4.8.5	Parameters in INTEGER Numbers	156
4.8.6	Case Study: Multiple Products	156
4.9	Operations with Algebraic Data	159
4.10	Operations with Arrays	162
4.10.1	BLAS	163
4.11	Operations with Analytic Data	164
4.11.1	Representation of Functions	164
4.11.2	Implementation of Functions	165
4.11.3	Operations with Functions	167
4.11.4	Functions as Results	171
5	Numerical Algorithms	172
5.1	The Intuitive Notion of an Algorithm	172
5.2	Properties of Algorithms	174
5.2.1	Abstraction	175
5.2.2	Generality	175

5.2.3	Finiteness	175
5.2.4	Termination	175
5.2.5	Deterministic Algorithms	177
5.2.6	Determinate Algorithms	177
5.3	Existence of Algorithms	178
5.3.1	Precise Definitions of “Algorithm”	179
5.3.2	Computable Functions	179
5.4	Practical Solvability of Problems	181
5.5	Complexity of Algorithms	181
5.5.1	Abstract Computer Models	183
5.5.2	Theoretical Execution Cost	184
5.5.3	Asymptotic Complexity of Algorithms	185
5.5.4	Problem Complexity	186
5.5.5	Case Study: Multiplication of Matrices	187
5.5.6	Practical Effort Determination	191
5.6	Representation of Algorithms	194
5.6.1	Fortran 90	194
5.6.2	Pseudocode	195
5.7	Influence of Rounding Errors on Numerical Algorithms	196
5.7.1	Arithmetic Algorithms	196
5.7.2	Implementation of Arithmetic Algorithms	199
5.7.3	Error Propagation	200
5.7.4	Error Propagation Analysis	201
5.8	Case Study: Floating-Point Summation	210
5.8.1	Pairwise Summation	212
5.8.2	Compensated Summation	213
5.8.3	Comparison of Summation Methods	214
5.8.4	Ascending Summation	215
6	Numerical Programs	219
6.1	The Quality of Numerical Programs	219
6.1.1	Reliability	219
6.1.2	Portability	224
6.1.3	Efficiency	226
6.2	Reasons for Poor Efficiency	229
6.2.1	Lack of Parallelism	229
6.2.2	Lack of Locality of Reference	232
6.2.3	Inadequate Memory Access Patterns	233
6.2.4	Overhead	234
6.3	The Measurement of Performance Indices	235
6.3.1	Measurement of the Workload	236
6.3.2	Measurement of the Time	238
6.3.3	Profiling	243
6.3.4	Spotting Performance Decreasing Factors	246
6.4	Performance Optimization	247

- 6.5 Architecture Independent Optimizations 248
- 6.6 Loop Optimizations 249
 - 6.6.1 Loop Unrolling 249
 - 6.6.2 Unrolling Nested Loops 252
 - 6.6.3 Loop Fusion 253
 - 6.6.4 The Elimination of Loop Branches 254
 - 6.6.5 Associative Transformations 256
 - 6.6.6 Loop Interchanges 257
- 6.7 Blocked Memory Access 258
 - 6.7.1 Hierarchical Blocking 261
- 6.8 Case Study: Multiplication of Matrices 262
 - 6.8.1 Loop Interchanges 263
 - 6.8.2 Loop Unrolling 264
 - 6.8.3 Blocking 266
 - 6.8.4 Block Copying 267
 - 6.8.5 Blocking, Copying and Loop Unrolling 269
 - 6.8.6 Optimizing System Software 269
- 7 Available Numerical Software 272**
 - 7.1 The Cost of Software 272
 - 7.2 Sources of Numerical Software 274
 - 7.2.1 Numerical Application Software 274
 - 7.2.2 Printed Programs 275
 - 7.2.3 Numerical Software Libraries 276
 - 7.2.4 Numerical Software Packages 278
 - 7.2.5 References to Software in this Book 280
 - 7.3 Software and the Internet 281
 - 7.3.1 The Internet 282
 - 7.3.2 Communication in the Internet, E-Mail 284
 - 7.3.3 Forums for Discussion on the Internet 285
 - 7.3.4 Resource Sharing on the Internet 285
 - 7.3.5 Finding Software in the Internet 291
 - 7.3.6 Internet Front Ends 292
 - 7.3.7 NETLIB 293
 - 7.3.8 eLib 295
 - 7.3.9 GAMS 295
 - 7.4 Interactive Multifunctional Systems 295
 - 7.4.1 Exploratory Systems 295
 - 7.4.2 Numerical Systems 296
 - 7.4.3 Symbolic Systems 297
 - 7.4.4 Simulation Systems 297
 - 7.5 Problem Solving Environments 298
 - 7.5.1 Available Problem Solving Environments 299
 - 7.6 Case Study: Software for Elliptic PDEs 300
 - 7.6.1 Problem Classification 301

7.6.2	Software Packages for Elliptic Problems	302
7.6.3	Numerical Program Library Sections	305
7.6.4	TOMS Programs	306
8	Using Approximation in Mathematical Model Building	308
8.1	Analytic Models	308
8.1.1	Elementary Functions as Models	309
8.1.2	Algorithms Used as Mathematical Models	311
8.2	Information and Data	312
8.2.1	Obtaining Algebraic Data from Discrete Information . .	312
8.2.2	Obtaining Analytic Data from Continuous Information .	312
8.2.3	The Discretization of Continuous Information	314
8.2.4	The Homogenization of Discrete Data	316
8.3	Discrete Approximation	317
8.3.1	Discrete Approximation Data	317
8.3.2	Interpolation	319
8.3.3	Case Study: Water Resistance of Vessels	319
8.4	Function Approximation	321
8.4.1	Nonadaptive Discretization	322
8.4.2	Adaptive Discretization	322
8.4.3	Homogenization Algorithms	323
8.4.4	Additional Information	325
8.5	Choosing a Model Function	326
8.5.1	Uniform or Piecewise Approximation	326
8.5.2	Linear Approximation	327
8.5.3	Nonlinear Approximation	329
8.5.4	Global or Local Approximation	330
8.5.5	Continuity and Differentiability	332
8.5.6	Condition	333
8.5.7	Invariance under Scaling	334
8.5.8	Constraints	335
8.5.9	Appearance	337
8.6	Choice of the Distance Function	339
8.6.1	Mathematical Foundations	339
8.6.2	Norms for Finite-Dimensional Spaces	341
8.6.3	Norms for Infinite-Dimensional Spaces	343
8.6.4	Weighted Norms	343
8.6.5	Hamming Distance	344
8.6.6	Robust Distance Functions	344
8.6.7	Orthogonal Approximation	347
8.7	Transformation of the Problem	350
8.7.1	Ordinate Transformation	350
8.7.2	Curves	351

9 Interpolation 353

9.1 Interpolation Problems 353

9.1.1 Choosing a Class of Functions 354

9.1.2 Determination of the Parameters of an Interpolation
Function 354

9.1.3 Manipulation of the Interpolation Function 355

9.2 Mathematical Foundations 356

9.2.1 The General Interpolation Problem 356

9.2.2 Interpolation of Function Values 360

9.3 Univariate Polynomial Interpolation 361

9.3.1 Univariate Polynomials 361

9.3.2 Representation Forms of Univariate Polynomials 362

9.3.3 The Calculation of Coefficients 367

9.3.4 The Evaluation of Polynomials 369

9.3.5 Error and Convergence Behavior 373

9.3.6 Algorithm Error in Polynomial Interpolation 374

9.3.7 The Convergence of Interpolation Polynomials 377

9.3.8 The Conditioning of Polynomial Interpolation 386

9.3.9 Choosing Interpolation Nodes 390

9.3.10 Hermite Interpolation 393

9.4 Univariate, Piecewise, Polynomial Interpolation 394

9.4.1 The Accuracy of the Approximation 396

9.4.2 Evaluation 397

9.5 Polynomial Splines 397

9.5.1 Oscillations and Sensitivity to Perturbations 399

9.5.2 The Representation of Polynomial Splines 401

9.6 B-Splines 403

9.6.1 Choice of the B-Spline Break Points 406

9.6.2 B-Splines in Graphical Data Processing 407

9.6.3 Software for B-Splines 411

9.7 Cubic Spline Interpolation 412

9.7.1 Boundary Conditions 413

9.7.2 Extremal Property 414

9.7.3 Error and Convergence Behavior 415

9.7.4 The Calculation of Coefficients 415

9.7.5 The Evaluation of Spline Functions 416

9.7.6 Condition 416

9.8 Splines Without Undesirable Oscillations 419

9.8.1 Exponential Splines 421

9.8.2 ν -Splines 422

9.8.3 The Akima Sub spline Interpolation 426

9.9 Multivariate Interpolation 429

9.9.1 Tensor Product Interpolation 430

9.9.2 Triangulation 431

9.10 Multivariate Polynomial Interpolation 433

9.11	Multivariate (Sub-) Spline Interpolation	435
9.11.1	Tensor Product Spline Functions	437
9.11.2	Polynomial Interpolation on Triangles	437
9.12	Related Problems and Methods	438
Glossary of Notation		440
Bibliography		443
Author Index		460
Subject Index		466