

Also available → a diskette version with FORTRAN
and C languages source codes



Numerical Methods

All Computer programs in
FORTRAN 77/90

C Language conversion of all
programs in an appendix

E Balagurusamy

Contents

<i>Preface</i>	<i>v</i>
1. Introduction to Numerical Computing	1
1.1 Introduction	1
1.2 Numeric Data	2
1.3 Analog Computing	2
1.4 Digital Computing	3
1.5 Process of Numerical Computing	3
1.6 Characteristics of Numerical Computing	8
<i>Accuracy</i>	8
<i>Rate of convergence</i>	8
<i>Numerical stability</i>	8
<i>Efficiency</i>	9
1.7 Computational Environment	9
1.8 New Trends in Numerical Computing	9
1.9 Mathematical Background	10
1.10 Summary	10
<i>Key terms</i>	10
<i>Review questions</i>	10
2. Introduction to Computers and Computing Concepts	12
2.1 Introduction	12
2.2 Evolution of Numerical Computing and Computers	14
<i>Modern computers</i>	15
<i>Fifth generation computers</i>	16
2.3 Types of Computers	17
<i>Principles of operation</i>	17
<i>Applications</i>	18
<i>Size and capability</i>	18
2.4 Computing Concepts	20

- 2.5 Computer Organisation 21
 - Input devices* 21
 - Processing units* 22
 - Output devices* 22
 - External storage devices* 23
- 2.6 Driving the Computer: The Software 24
 - Operating system* 24
 - Utility programs* 25
 - Language processors* 26
 - Application programs* 26
- 2.7 Programming Languages 27
 - Machine language* 27
 - Assembly language* 27
 - Procedure-oriented language (POL)* 28
 - Common high-level languages* 29
- 2.8 Interactive Computing 30
- 2.9 Problem Solving and Algorithms 30
- 2.10 Flow Charting 32
- 2.11 Structuring the Logic 33
- 2.12 Using the Computer 35
- 2.13 Summary 36
 - Key terms* 36
 - Review questions* 37

3. Computer Codes and Arithmetic

40

- 3.1 Introduction 40
- 3.2 Decimal System 41
- 3.3 Binary System 42
- 3.4 Hexadecimal System 42
- 3.5 Octal System 44
- 3.6 Conversion of Numbers 45
 - Non-decimal system to decimal system* 45
 - Decimal system to non-decimal system* 46
 - Octal and hexadecimal conversion* 48
- 3.7 Representation of Numbers 49
 - Integer representation* 50
 - Floating-point representation* 51
- 3.8 Computer Arithmetic 52
 - Integer arithmetic* 52
 - Floating-point arithmetic* 53
- 3.9 Errors in Arithmetic 55
- 3.10 Laws of Arithmetic 57
- 3.11 Summary 58
 - Key terms* 58
 - Review questions* 59
 - Review exercises* 60

4. Approximations and Errors in Computing	61
4.1 Introduction	61
4.2 Significant Digits	62
4.3 Inherent Errors	64
<i>Data errors</i>	64
<i>Conversion errors</i>	64
4.4 Numerical Errors	65
<i>Roundoff errors</i>	65
<i>Chopping</i>	65
<i>Symmetric roundoff</i>	66
<i>Truncation errors</i>	67
4.5 Modelling Errors	69
4.6 Blunders	69
4.7 Absolute and Relative Errors	70
4.8 Machine Epsilon	71
4.9 Error Propagation	73
<i>Addition and subtraction</i>	73
<i>Multiplication</i>	73
<i>Division</i>	74
<i>Sequence of computations</i>	76
<i>Addition of a chain of numbers</i>	77
<i>Polynomial functions</i>	79
4.10 Conditioning and Stability	80
4.11 Convergence of Iterative Processes	86
4.12 Error Estimation	87
4.13 Minimising the Total Error	88
4.14 Pitfalls and Precautions	88
4.15 Summary	89
<i>Key terms</i>	90
<i>Review questions</i>	90
<i>Review exercises</i>	91
5. FORTRAN 77 Overview	93
5.1 Need and Scope	93
5.2 A Sample Program	93
5.3 FORTRAN Constants	97
5.4 FORTRAN Variables	98
5.5 Subscripted Variables	99
5.6 Input/Output Statements	100
5.7 Computations	101
<i>Mixed-mode expressions</i>	102
5.8 Control of Execution	103
<i>Block if-else structure</i>	103
<i>Relational expressions</i>	104
<i>Logical expressions</i>	105
<i>Do-while structure</i>	106

5.9	Subprograms	109
	<i>Function subprograms</i>	109
	<i>Subroutine subprogram</i>	110
5.10	Intrinsic Functions	112
5.11	Debugging, Testing and Documentation	113
5.12	Summary	114
	<i>Key terms</i>	114
	<i>Review questions</i>	115
	<i>Review exercises</i>	116
6.	Roots of Nonlinear Equations	
6.1	Introduction	121
	<i>Algebraic equations</i>	122
	<i>Polynomial equations</i>	122
	<i>Transcendental equations</i>	122
6.2	Methods of Solution	123
6.3	Iterative Methods	124
6.4	Starting and Stopping an Iterative Process	125
	<i>Starting the process</i>	125
	<i>Stopping criterion</i>	127
6.5	Evaluation of Polynomials	127
	<i>Program POLY</i>	129
6.6	Bisection Method	131
	<i>Convergence of bisection method</i>	134
	<i>Program BISECT</i>	134
6.7	False Position Method	138
	<i>False position formula</i>	138
	<i>False position algorithm</i>	139
	<i>Convergence of false position method</i>	140
	<i>Program FALSE</i>	141
6.8	Newton-Raphson Method	145
	<i>Newton-Raphson algorithm</i>	146
	<i>Convergence of Newton-Raphson method</i>	147
	<i>Program NEWTON</i>	148
	<i>Limitations of Newton-Raphson method</i>	151
6.9	Secant Method	151
	<i>Secant algorithm</i>	153
	<i>Convergence of secant method</i>	155
	<i>Program SECANT</i>	157
6.10	Fixed-Point Method	160
	<i>Convergence of fixed point iteration</i>	163
	<i>Program FIXEDP</i>	164
6.11	Determining all Possible Roots	166
6.12	Systems of Nonlinear Equations	168
	<i>Fixed point method</i>	168
	<i>Newton-Raphson method</i>	170
6.13	Roots of Polynomials	173
	<i>Multiple roots</i>	174

	<i>Deflation and synthetic division</i>	175
	<i>Complex roots</i>	176
	<i>Purification of roots</i>	177
6.14	Multiple Roots by Newton's Method	178
	<i>Program MULTIR</i>	178
6.15	Complex Roots by Bairstow Method	183
	<i>Program COMPR</i>	188
6.16	Muller's Method	195
	<i>Complex roots</i>	199
	<i>Multiple roots</i>	199
	<i>Program MULLER</i>	199
6.17	Summary	199
	<i>Key terms</i>	200
	<i>Review questions</i>	200
	<i>Review exercises</i>	202
	<i>Programming projects</i>	205
7.	Direct Solution of Linear Equations	206
7.1	Need and Scope	206
7.2	Existence of Solution	207
	<i>Unique solution</i>	208
	<i>No solution</i>	208
	<i>No unique solution</i>	209
	<i>Ill-conditioned systems</i>	209
7.3	Solution by Elimination	209
7.4	Basic Gauss Elimination Method	212
	<i>Computational effort</i>	215
	<i>Program LEG1</i>	216
7.5	Gauss Elimination with Pivoting	219
	<i>Program LEG2</i>	222
7.6	Gauss-Jordan Method	228
	<i>Computational effort</i>	229
7.7	Triangular Factorization Methods	230
	<i>Dolittle algorithm</i>	231
	<i>Program DOLIT</i>	235
	<i>Crout algorithm</i>	240
	<i>Cholesky method</i>	241
7.8	Round-off Errors and Refinement	242
7.9	Ill-Conditioned Systems	244
7.10	Matrix Inversion Method	245
	<i>Computing matrix inverse</i>	246
	<i>Condition number</i>	246
7.11	Summary	247
	<i>Key terms</i>	247
	<i>Review questions</i>	248
	<i>Review exercises</i>	249
	<i>Programming projects</i>	251

8. Iterative Solution of Linear Equations

- 8.1 Need and Scope 252
- 8.2 Jacobi Iteration Method 252
 - Program JACIT* 255
- 8.3 Gauss-Seidel Method 259
 - Algorithm* 261
 - Program GASIT* 262
- 8.4 Method of Relaxation 266
- 8.5 Convergence of Iteration Methods 267
 - Condition for convergence* 267
 - Rate of convergence* 268
- 8.6 Summary 272
 - Key terms* 272
 - Review questions* 272
 - Review exercises* 273
 - Programming projects* 274

9. Curve Fitting: Interpolation

- 9.1 Introduction 275
- 9.2 Polynomial Forms 277
- 9.3 Linear Interpolation 279
- 9.4 Lagrange Interpolation Polynomial 281
 - Program LAGRAN* 284
- 9.5 Newton Interpolation Polynomial 286
- 9.6 Divided Difference Table 290
 - Program NEWINT* 292
- 9.7 Interpolation with Equidistant Points 294
 - Forward difference table* 296
 - Backward difference table* 298
- 9.8 Spline Interpolation 299
 - Cubic splines* 302
 - Algorithm* 307
 - Program SPLINE* 308
 - Equidistant knots* 312
- 9.9 Chebyshev Interpolation Polynomial 314
 - Chebyshev points* 314
 - Chebyshev polynomials* 315
- 9.10 Summary 315
 - Key terms* 316
 - Review questions* 317
 - Review exercises* 317
 - Programming projects* 321

10. Curve Fitting: Regression

- 10.1 Introduction 323
- 10.2 Fitting Linear Equations 324
 - Least squares regression* 325
 - Algorithm* 327
 - Program LINREG* 327

10.3	Fitting Transcendental Equations	329	
10.4	Fitting a Polynomial Function	333	
	<i>Algorithm for polynomial fit</i>	336	
	<i>Program POLREG</i>	337	
10.5	Multiple Linear Regression	341	
10.6	Ill-Conditioning in Least-Squares Methods	342	
10.7	Summary	343	
	<i>Key terms</i>	343	
	<i>Review questions</i>	343	
	<i>Review exercises</i>	344	
	<i>Programming projects</i>	346	
11.	Numerical Differentiation		347
11.1	Need and Scope	347	
11.2	Differentiating Continuous Functions	348	
	<i>Forward difference quotient</i>	348	
	<i>Central difference quotient</i>	349	
	<i>Error analysis</i>	351	
	<i>Higher-order derivatives</i>	354	
11.3	Differentiating Tabulated Functions	355	
	<i>Error analysis</i>	357	
	<i>Higher-order derivatives</i>	358	
11.4	Difference Tables	360	
11.5	Richardson Extrapolation	362	
11.6	Summary	364	
	<i>Key terms</i>	365	
	<i>Review questions</i>	365	
	<i>Review exercises</i>	366	
	<i>Programming projects</i>	368	
12.	Numerical Integration		369
12.1	Need and Scope	369	
12.2	Newton-Cotes Methods	371	
12.3	Trapezoidal Rule	372	
	<i>Error analysis</i>	373	
	<i>Composite trapezoidal rule</i>	374	
	<i>Program TRAPE1</i>	377	
12.4	Simpson's 1/3 Rule	379	
	<i>Error analysis</i>	380	
	<i>Composite Simpson's 1/3 rule</i>	382	
	<i>Program SIMS1</i>	383	
12.5	Simpson's 3/8 Rule	385	
12.6	Higher Order Rules	387	
12.7	Romberg Integration	388	
	<i>Program ROMBRG</i>	392	
12.8	Gaussian Integration	394	
	<i>Changing limits of integration</i>	397	
	<i>Higher-order Gaussian formulae</i>	399	

- 12.9 Summary 401
 - Key terms 401
 - Review questions 402
 - Review exercises 403
 - Programming projects 406

13. Numerical Solution of Ordinary Differential Equations

- 13.1 Need and Scope 408
 - Number of independent variables 410
 - Order of equations 410
 - Degree of equations 410
 - Linear and nonlinear equations 411
 - General and particular solutions 411
 - Initial value problems 412
 - One-step and multistep methods 412
 - Scope 412
- 13.2 Taylor Series Method 413
 - Improving accuracy 414
 - Picard's method 417
- 13.3 Euler's Method 419
 - Accuracy of Euler's method 421
 - Program EULER 423
- 13.4 Heun's Method 425
 - Error analysis 428
 - Program HEUN 429
- 13.5 Polygon Method 432
 - Program POLYGN 434
- 13.6 Runge-Kutta Methods 436
 - Determination of weights 437
 - Fourth-order Runge-Kutta methods 439
 - Program RUNGE4 440
- 13.7 Accuracy of One-step Methods 442
- 13.8 Multistep Methods 444
 - Milne-Simpson method 445
 - Program MILSIM 447
 - Adams-Bashforth-Moulton method 450
- 13.9 Accuracy of Multistep Methods 451
 - Milne-Simpson method 451
 - Adams method 452
 - Modifiers 452
- 13.10 Systems of Differential Equations 454
- 13.11 Higher-Order Equations 456
- 13.12 Summary 457
 - Key terms 458
 - Review questions 458
 - Review exercises 460
 - Programming projects 463

14. Boundary-value and Eigenvalue Problems	464
14.1 Need and Scope	464
14.2 Shooting Method	465
14.3 Finite Difference Method	469
14.4 Solving Eigenvalue Problems	472
14.5 Polynomial Method	473
<i>The Fadeev-Leverrier method</i>	474
<i>Evaluating the eigenvalues</i>	475
<i>Determining the eigenvectors</i>	476
<i>Computing algorithm</i>	477
14.6 Power Method	477
14.7 Summary	479
<i>Key terms</i>	480
<i>Review questions</i>	480
<i>Review exercises</i>	481
<i>Programming projects</i>	482
15. Solution of Partial Differential Equations	483
15.1 Need and Scope	483
15.2 Deriving Difference Equations	484
15.3 Elliptic Equations	486
<i>Laplace's equation</i>	486
<i>Liebmann's iterative method</i>	489
<i>Poisson's equation</i>	490
15.4 Parabolic Equations	492
<i>Solution of heat equation</i>	493
<i>Bender-Schmidt method</i>	494
<i>The Crank-Nicholson method</i>	495
15.5 Hyperbolic Equations	497
<i>Solution of hyperbolic equations</i>	498
<i>Starting values</i>	499
15.6 Summary	500
<i>Key terms</i>	501
<i>Review questions</i>	501
<i>Review exercises</i>	502
<i>Programming projects</i>	504
Appendix A: Solution of Linear Systems by Matrix Methods	505
A.1 Overview of Matrices	505
A.2 Solution of Linear Systems by Determinants	509
A.3 Solution of Linear Systems by Matrix Inversion	510
A.4 Gauss-Jordan Matrix Inversion	513
Appendix B: Solution of Polynomials by Graeffe's Root Squaring Method	516

Appendix C: Difference Operators and Central Difference Interpolation Formulae	520
C.1 Introduction	520
C.2 Finite Differences	520
C.3 Difference Operators	522
C.4 Relations between the Operators	523
C.5 Central Difference Interpolation Formulae	525
Appendix D: C Programs	531
D.1 Introduction	531
D.2 FORTRAN to C Conversion	533
Appendix E: Bibliography	600
E.1 Numerical Computing	600
E.2 Programming	601
Index	602