

Contents

Chapter I. Classical Mathematical Theory

I.1	Terminology	2
I.2	The Oldest Differential Equations	4
	Newton	4
	Leibniz and the Bernoulli Brothers	6
	Variational Calculus	7
	Clairaut	9
	Exercises	10
I.3	Elementary Integration Methods	12
	First Order Equations	12
	Second Order Equations	13
	Exercises	14
I.4	Linear Differential Equations	16
	Equations with Constant Coefficients	16
	Variation of Constants	18
	Exercises	19
I.5	Equations with Weak Singularities	20
	Linear Equations	20
	Nonlinear Equations	23
	Exercises	24
I.6	Systems of Equations	26
	The Vibrating String and Propagation of Sound	26
	Fourier	29
	Lagrangian Mechanics	30
	Hamiltonian Mechanics	32
	Exercises	34
I.7	A General Existence Theorem	35
	Convergence of Euler's Method	35
	Existence Theorem of Peano	41
	Exercises	43
I.8	Existence Theory using Iteration Methods and Taylor Series	44
	Picard-Lindelöf Iteration	45
	Taylor Series	46
	Recursive Computation of Taylor Coefficients	47
	Exercises	49

I.9	Existence Theory for Systems of Equations	51
	Vector Notation	52
	Subordinate Matrix Norms	53
	Exercises	55
I.10	Differential Inequalities	56
	Introduction	56
	The Fundamental Theorems	57
	Estimates Using One-Sided Lipschitz Conditions	60
	Exercises	62
I.11	Systems of Linear Differential Equations	64
	Resolvent and Wronskian	65
	Inhomogeneous Linear Equations	66
	The Abel-Liouville-Jacobi-Ostrogradskii Identity	66
	Exercises	67
I.12	Systems with Constant Coefficients	69
	Linearization	69
	Diagonalization	69
	The Schur Decomposition	70
	Numerical Computations	72
	The Jordan Canonical Form	73
	Geometric Representation	77
	Exercises	78
I.13	Stability	80
	Introduction	80
	The Routh-Hurwitz Criterion	81
	Computational Considerations	85
	Liapunov Functions	86
	Stability of Nonlinear Systems	87
	Stability of Non-Autonomous Systems	88
	Exercises	89
I.14	Derivatives with Respect to Parameters and Initial Values ..	92
	The Derivative with Respect to a Parameter	93
	Derivatives with Respect to Initial Values	95
	The Nonlinear Variation-of-Constants Formula	96
	Flows and Volume-Preserving Flows	97
	Canonical Equations and Symplectic Mappings	100
	Exercises	104
I.15	Boundary Value and Eigenvalue Problems	105
	Boundary Value Problems	105
	Sturm-Liouville Eigenvalue Problems	107
	Exercises	110
I.16	Periodic Solutions, Limit Cycles, Strange Attractors	111
	Van der Pol's Equation	111
	Chemical Reactions	115
	Limit Cycles in Higher Dimensions, Hopf Bifurcation	117
	Strange Attractors	120
	The Ups and Downs of the Lorenz Model	123
	Feigenbaum Cascades	124
	Exercises	126

Chapter II. Runge-Kutta and Extrapolation Methods

II.1	The First Runge-Kutta Methods	132
	General Formulation of Runge-Kutta Methods	134
	Discussion of Methods of Order 4	135
	"Optimal" Formulas	139
	Numerical Example	140
	Exercises	141
II.2	Order Conditions for Runge-Kutta Methods	143
	The Derivatives of the True Solution	145
	Conditions for Order 3	145
	Trees and Elementary Differentials	145
	The Taylor Expansion of the True Solution	148
	Faà di Bruno's Formula	149
	The Derivatives of the Numerical Solution	151
	The Order Conditions	153
	Exercises	154
II.3	Error Estimation and Convergence for RK Methods	156
	Rigorous Error Bounds	156
	The Principal Error Term	158
	Estimation of the Global Error	159
	Exercises	163
II.4	Practical Error Estimation and Step Size Selection	164
	Richardson Extrapolation	164
	Embedded Runge-Kutta Formulas	165
	Automatic Step Size Control	167
	Starting Step Size	169
	Numerical Experiments	170
	Exercises	172
II.5	Explicit Runge-Kutta Methods of Higher Order	173
	The Butcher Barriers	173
	6-Stage, 5th Order Processes	175
	Embedded Formulas of Order 5	176
	Higher Order Processes	179
	Embedded Formulas of High Order	180
	An 8th Order Embedded Method	181
	Exercises	185
II.6	Dense Output, Discontinuities, Derivatives	188
	Dense Output	188
	Continuous Dormand & Prince Pairs	191
	Dense Output for DOP853	194
	Event Location	195
	Discontinuous Equations	196
	Numerical Computation of Derivatives with Respect to Initial Values and Parameters	200
	Exercises	202
II.7	Implicit Runge-Kutta Methods	204
	Existence of a Numerical Solution	206
	The Methods of Kuntzmann and Butcher of Order 2s	208
	IRK Methods Based on Lobatto Quadrature	210

	Collocation Methods	211
	Exercises	214
II.8	Asymptotic Expansion of the Global Error	216
	The Global Error	216
	Variable h	218
	Negative h	219
	Properties of the Adjoint Method	220
	Symmetric Methods	221
	Exercises	223
II.9	Extrapolation Methods	224
	Definition of the Method	224
	The Aitken - Neville Algorithm	226
	The Gragg or GBS Method	228
	Asymptotic Expansion for Odd Indices	231
	Existence of Explicit RK Methods of Arbitrary Order	232
	Order and Step Size Control	233
	Dense Output for the GBS Method	237
	Control of the Interpolation Error	240
	Exercises	241
II.10	Numerical Comparisons	244
	Problems	244
	Performance of the Codes	249
	A "Stretched" Error Estimator for DOP853	254
	Effect of Step-Number Sequence in ODEX	256
II.11	Parallel Methods	257
	Parallel Runge-Kutta Methods	258
	Parallel Iterated Runge-Kutta Methods	259
	Extrapolation Methods	261
	Increasing Reliability	261
	Exercises	263
II.12	Composition of B-Series	264
	Composition of Runge-Kutta Methods	264
	B-Series	266
	Order Conditions for Runge-Kutta Methods	269
	Butcher's "Effective Order"	270
	Exercises	272
II.13	Higher Derivative Methods	274
	Collocation Methods	275
	Hermite-Obreschkoff Methods	277
	Fehlberg Methods	278
	General Theory of Order Conditions	280
	Exercises	281
II.14	Numerical Methods for Second Order Differential Equations	283
	Nyström Methods	284
	The Derivatives of the Exact Solution	286
	The Derivatives of the Numerical Solution	288
	The Order Conditions	290
	On the Construction of Nyström Methods	291
	An Extrapolation Method for $y'' = f(x, y)$	294
	Problems for Numerical Comparisons	296

Performance of the Codes	298
Exercises	300
II.15 P-Series for Partitioned Differential Equations	302
Derivatives of the Exact Solution, P-Trees	303
P-Series	306
Order Conditions for Partitioned Runge-Kutta Methods	307
Further Applications of P-Series	308
Exercises	311
II.16 Symplectic Integration Methods	312
Symplectic Runge-Kutta Methods	315
An Example from Galactic Dynamics	319
Partitioned Runge-Kutta Methods	326
Symplectic Nyström Methods	330
Conservation of the Hamiltonian; Backward Analysis	333
Exercises	337
II.17 Delay Differential Equations	339
Existence	339
Constant Step Size Methods for Constant Delay	341
Variable Step Size Methods	342
Stability	343
An Example from Population Dynamics	345
Infectious Disease Modelling	347
An Example from Enzyme Kinetics	248
A Mathematical Model in Immunology	349
Integro-Differential Equations	351
Exercises	352

Chapter III. Multistep Methods and General Linear Methods

III.1 Classical Linear Multistep Formulas	356
Explicit Adams Methods	357
Implicit Adams Methods	359
Numerical Experiment	361
Explicit Nyström Methods	362
Milne-Simpson Methods	363
Methods Based on Differentiation (BDF)	364
Exercises	366
III.2 Local Error and Order Conditions	368
Local Error of a Multistep Method	368
Order of a Multistep Method	370
Error Constant	372
Irreducible Methods	374
The Peano Kernel of a Multistep Method	375
Exercises	377
III.3 Stability and the First Dahlquist Barrier	378
Stability of the BDF-Formulas	380
Highest Attainable Order of Stable Multistep Methods	383
Exercises	387

III.4 Convergence of Multistep Methods	391
Formulation as One-Step Method	393
Proof of Convergence	395
Exercises	396
III.5 Variable Step Size Multistep Methods	397
Variable Step Size Adams Methods	397
Recurrence Relations for $g_j(n)$, $\Phi_j(n)$ and $\Phi_j^*(n)$	399
Variable Step Size BDF	400
General Variable Step Size Methods and Their Orders	401
Stability	402
Convergence	407
Exercises	409
III.6 Nordsieck Methods	410
Equivalence with Multistep Methods	412
Implicit Adams Methods	417
BDF-Methods	419
Exercises	420
III.7 Implementation and Numerical Comparisons	421
Step Size and Order Selection	421
Some Available Codes	423
Numerical Comparisons	427
III.8 General Linear Methods	430
A General Integration Procedure	431
Stability and Order	436
Convergence	438
Order Conditions for General Linear Methods	441
Construction of General Linear Methods	443
Exercises	445
III.9 Asymptotic Expansion of the Global Error	448
An Instructive Example	448
Asymptotic Expansion for Strictly Stable Methods (8.4)	450
Weakly Stable Methods	454
The Adjoint Method	457
Symmetric Methods	459
Exercises	460
III.10 Multistep Methods for Second Order Differential Equations	461
Explicit Störmer Methods	462
Implicit Störmer Methods	464
Numerical Example	465
General Formulation	467
Convergence	468
Asymptotic Formula for the Global Error	471
Rounding Errors	472
Exercises	473
Appendix. Fortran Codes	475
Driver for the Code DOPRI5	475
Subroutine DOPRI5	477
Subroutine DOP853	481
Subroutine ODEX	482

Subroutine ODEX2	484
Driver for the Code RETARD	486
Subroutine RETARD	488
Bibliography	491
Symbol Index	521
Subject Index	523