

# Contents

## Chapter I. Classical Mathematical Theory

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

<b>I.9</b>	<b>Existence Theory for Systems of Equations</b>	51
	Vector Notation	52
	Subordinate Matrix Norms	53
	Exercises	55
<b>I.10</b>	<b>Differential Inequalities</b>	56
	Introduction	56
	The Fundamental Theorems	57
	Estimates Using One-Sided Lipschitz Conditions	60
	Exercises	62
<b>I.11</b>	<b>Systems of Linear Differential Equations</b>	64
	Resolvent and Wronskian	65
	Inhomogeneous Linear Equations	66
	The Abel-Liouville-Jacobi-Ostrogradskii Identity	66
	Exercises	67
<b>I.12</b>	<b>Systems with Constant Coefficients</b>	69
	Linearization	69
	Diagonalization	69
	The Schur Decomposition	70
	Numerical Computations	72
	The Jordan Canonical Form	73
	Geometric Representation	77
	Exercises	78
<b>I.13</b>	<b>Stability</b>	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
<b>I.14</b>	<b>Derivatives with Respect to Parameters and Initial Values</b>	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
<b>I.15</b>	<b>Boundary Value and Eigenvalue Problems</b>	105
	Boundary Value Problems	105
	Sturm-Liouville Eigenvalue Problems	107
	Exercises	110
<b>I.16</b>	<b>Periodic Solutions, Limit Cycles, Strange Attractors</b>	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

<b>II.1</b>	<b>The First Runge-Kutta Methods</b>	132
	General Formulation of Runge-Kutta Methods	134
	Discussion of Methods of Order 4	135
	“Optimal” Formulas	139
	Numerical Example	140
	Exercises	141
<b>II.2</b>	<b>Order Conditions for Runge-Kutta Methods</b>	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
<b>II.3</b>	<b>Error Estimation and Convergence for RK Methods</b>	156
	Rigorous Error Bounds	156
	The Principal Error Term	158
	Estimation of the Global Error	159
	Exercises	163
<b>II.4</b>	<b>Practical Error Estimation and Step Size Selection</b>	164
	Richardson Extrapolation	164
	Embedded Runge-Kutta Formulas	165
	Automatic Step Size Control	167
	Starting Step Size	169
	Numerical Experiments	170
	Exercises	172
<b>II.5</b>	<b>Explicit Runge-Kutta Methods of Higher Order</b>	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
<b>II.6</b>	<b>Dense Output, Discontinuities, Derivatives</b>	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
<b>II.7</b>	<b>Implicit Runge-Kutta Methods</b>	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
<b>II.8 Asymptotic Expansion of the Global Error .....</b>	<b>216</b>
The Global Error .....	216
Variable $h$ .....	218
Negative $h$ .....	219
Properties of the Adjoint Method .....	220
Symmetric Methods .....	221
Exercises .....	223
<b>II.9 Extrapolation Methods.....</b>	<b>224</b>
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
<b>II.10 Numerical Comparisons.....</b>	<b>244</b>
Problems .....	244
Performance of the Codes .....	249
A "Stretched" Error Estimator for DOP853 .....	254
Effect of Step-Number Sequence in ODEX .....	256
<b>II.11 Parallel Methods .....</b>	<b>257</b>
Parallel Runge-Kutta Methods .....	258
Parallel Iterated Runge-Kutta Methods .....	259
Extrapolation Methods .....	261
Increasing Reliability .....	261
Exercises .....	263
<b>II.12 Composition of B-Series .....</b>	<b>264</b>
Composition of Runge-Kutta Methods .....	264
B-Series .....	266
Order Conditions for Runge-Kutta Methods .....	269
Butcher's "Effective Order" .....	270
Exercises .....	272
<b>II.13 Higher Derivative Methods .....</b>	<b>274</b>
Collocation Methods .....	275
Hermite-Obreschkoff Methods .....	277
Fehlberg Methods .....	278
General Theory of Order Conditions .....	280
Exercises .....	281
<b>II.14 Numerical Methods for Second Order Differential Equations</b> .....	<b>283</b>
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
<b>II.15 P-Series for Partitioned Differential Equations .....</b>	<b>302</b>
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
<b>II.16 Symplectic Integration Methods .....</b>	<b>312</b>
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
<b>II.17 Delay Differential Equations .....</b>	<b>339</b>
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

<b>III.1 Classical Linear Multistep Formulas .....</b>	<b>356</b>
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
<b>III.2 Local Error and Order Conditions .....</b>	<b>368</b>
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
<b>III.3 Stability and the First Dahlquist Barrier .....</b>	<b>378</b>
Stability of the BDF-Formulas .....	380
Highest Attainable Order of Stable Multistep Methods .....	383
Exercises .....	387

<b>III.4 Convergence of Multistep Methods</b>	391
Formulation as One-Step Method	393
Proof of Convergence	395
Exercises	396
<b>III.5 Variable Step Size Multistep Methods</b>	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
<b>III.6 Nordsieck Methods</b>	410
Equivalence with Multistep Methods	412
Implicit Adams Methods	417
BDF-Methods	419
Exercises	420
<b>III.7 Implementation and Numerical Comparisons</b>	421
Step Size and Order Selection	421
Some Available Codes	423
Numerical Comparisons	427
<b>III.8 General Linear Methods</b>	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
<b>III.9 Asymptotic Expansion of the Global Error</b>	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
<b>III.10 Multistep Methods for Second Order Differential Equations</b>	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
<b>Appendix. Fortran Codes</b>	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
<b>Bibliography</b> .....	491
<b>Symbol Index</b> .....	521
<b>Subject Index</b> .....	523