

Contents

Preface	v
Preface	vii
Outline	xv
1 Time-Dependent Processes in Science and Engineering	1
1.1 Newton's Celestial Mechanics	4
1.2 Classical Molecular Dynamics	9
1.3 Chemical Reaction Kinetics	13
1.4 Electrical Circuits	22
Exercises	27
2 Existence and Uniqueness for Initial Value Problems	33
2.1 Global Existence and Uniqueness	34
2.2 Examples of Maximal Continuation	40
2.3 Structure of Nonunique Solutions	44
2.4 Weakly Singular Initial Value Problems	51
2.5 Singular Perturbation Problems	57
2.6 Quasilinear Differential-Algebraic Problems	60
Exercises	70
3 Condition of Initial Value Problems	75
3.1 Sensitivity Under Perturbations	76

3.1.1	Propagation Matrices	76
3.1.2	Condition Numbers	82
3.1.3	Perturbation Index of DAE Problems	86
3.2	Stability of ODEs	91
3.2.1	Stability Concept	92
3.2.2	Linear Autonomous ODEs	94
3.2.3	Stability of Fixed Points	102
3.3	Stability of Recursive Mappings	107
3.3.1	Linear Autonomous Recursions	107
3.3.2	Spectra of Rational Matrix Functions	113
	Exercises	115
4	One-Step Methods for Nonstiff IVPs	121
4.1	Convergence Theory	123
4.1.1	Consistency	124
4.1.2	Convergence	125
4.1.3	Concept of Stiffness	130
4.2	Explicit Runge-Kutta Methods	133
4.2.1	Concept of Runge-Kutta Methods	134
4.2.2	Classical Runge-Kutta Methods	139
4.2.3	Higher-Order Runge-Kutta Methods	145
4.2.4	Discrete Condition Numbers	154
4.3	Explicit Extrapolation Methods	158
4.3.1	Concept of Extrapolation Methods	159
4.3.2	Asymptotic Expansion of Discretization Error	163
4.3.3	Extrapolation of Explicit Midpoint Rule	168
4.3.4	Extrapolation of Störmer/Verlet Discretization	175
	Exercises	183
5	Adaptive Control of One-Step Methods	191
5.1	Local Accuracy Control	193
5.2	Control-Theoretic Analysis	197
5.2.1	Excursion to PID Controllers	197
5.2.2	Step-size Selection as Controller	200
5.3	Error Estimation	203
5.4	Embedded Runge-Kutta Methods	207
5.5	Local Versus Achieved Accuracy	213
	Exercises	217
6	One-Step Methods for Stiff ODE and DAE IVPs	219
6.1	Inheritance of Asymptotic Stability	222
6.1.1	Rational Approximation of Matrix Exponential	223
6.1.2	Stability Domains	225
6.1.3	Stability Concepts	233
6.1.4	Reversibility and Discrete Isometries	237

6.1.5	Extension to Nonlinear Problems	240
6.2	Implicit Runge-Kutta Methods	244
6.2.1	Stability Functions	251
6.2.2	Solution of Nonlinear Systems	254
6.3	Collocation Methods	258
6.3.1	Basic Idea of Collocation	259
6.3.2	Gauss and Radau Methods	267
6.3.3	Dissipative ODEs	271
6.3.4	Conservation of Quadratic First Integrals	277
6.4	Linearly Implicit One-Step Methods	280
6.4.1	Linearly Implicit Runge-Kutta Methods	280
6.4.2	Linearly Implicit Extrapolation Methods	284
6.4.3	Dynamic Elimination of Fast Modes	293
	Exercises	305
7	Multistep Methods for ODE and DAE IVPs	313
7.1	Multistep Methods on Equidistant Meshes	315
7.1.1	Consistency	319
7.1.2	Stability	323
7.1.3	Convergence	328
7.1.4	Discrete Condition Numbers	337
7.2	Inheritance of Asymptotic Stability	339
7.2.1	Weak Instability in Multistep Methods	341
7.2.2	Linear Stability in Stiff Problems	344
7.3	Direct Construction of Efficient Multistep Methods	348
7.3.1	Adams Methods for Nonstiff ODE Problems	348
7.3.2	BDF Methods for Stiff ODE and DAE Problems	356
7.4	Adaptive Control of Order and Step Size	362
7.4.1	Adams Methods on Variable Meshes	365
7.4.2	BDF Methods on Variable Meshes	367
7.4.3	Nordsieck Representation	376
	Exercises	384
8	Boundary Value Problems for ODEs	389
8.1	Sensitivity for Two-Point BVPs	390
8.1.1	Local Uniqueness	390
8.1.2	Condition Numbers	393
8.2	Initial Value Methods for Timelike BVPs	397
8.2.1	Shooting Method	397
8.2.2	Multiple Shooting Method	400
8.3	Cyclic Systems of Linear Equations	406
8.3.1	Discrete Condition Numbers	407
8.3.2	Algorithms	410
8.4	Global Discretization Methods for Spacelike BVPs	415
8.4.1	Elementary Finite Difference Methods	416

8.4.2	Adaptive Collocation Methods	423
8.5	More General Types of BVPs	426
8.5.1	Computation of Periodic Orbits	428
8.5.2	Parameter Identification in ODEs	434
8.6	Variational Problems	440
8.6.1	Classical Variational Problems	441
8.6.2	Optimal Control Problems	449
	Exercises	454
	References	461
	Software	475
	Index	477