

# Contents

## Chapter IV. Stiff Problems – One-Step Methods

<b>IV.1</b>	<b>Examples of Stiff Equations</b> .....	2
	Chemical Reaction Systems .....	3
	Electrical Circuits .....	4
	Diffusion .....	6
	A “Stiff” Beam .....	8
	High Oscillations .....	11
	Exercises .....	11
<b>IV.2</b>	<b>Stability Analysis for Explicit RK Methods</b> .....	15
	Stability Analysis for Euler’s Method .....	15
	Explicit Runge-Kutta Methods .....	16
	Extrapolation Methods .....	18
	Analysis of the Examples of IV.1 .....	18
	Automatic Stiffness Detection .....	21
	Step-Control Stability .....	24
	A PI Step Size Control .....	28
	Stabilized Explicit Runge-Kutta Methods .....	31
	Exercises .....	37
<b>IV.3</b>	<b>Stability Function of Implicit RK-Methods</b> .....	40
	The Stability Function .....	40
	$A$ -Stability .....	42
	$L$ -Stability and $A(\alpha)$ -Stability .....	44
	Numerical Results .....	46
	Stability Functions of Order $\geq s$ .....	47
	Padé Approximations to the Exponential Function .....	48
	Exercises .....	49
<b>IV.4</b>	<b>Order Stars</b> .....	51
	Introduction .....	51
	Order and Stability for Rational Approximations .....	56
	Stability of Padé Approximations .....	58
	Comparing Stability Domains .....	58
	Rational Approximations with Real Poles .....	61
	The Real-Pole Sandwich .....	62
	Multiple Real-Pole Approximations .....	67
	Exercises .....	70
<b>IV.5</b>	<b>Construction of Implicit Runge-Kutta Methods</b> .....	71
	Gauss Methods .....	71
	Radau IA and Radau IIA Methods .....	72

Lobatto IIIA, IIIB and IIIC Methods .....	75
The $W$ -Transformation .....	77
Construction of Implicit Runge-Kutta Methods .....	83
Stability Function .....	84
Positive Functions .....	86
Exercises .....	89
<b>IV.6 Diagonally Implicit RK Methods</b> .....	91
Order Conditions .....	91
Stiffly Accurate SDIRK Methods .....	92
The Stability Function .....	96
Multiple Real-Pole Approximations with $R(\infty)=0$ .....	98
Choice of Method .....	99
Exercises .....	100
<b>IV.7 Rosenbrock-Type Methods</b> .....	102
Derivation of the Method .....	102
Order Conditions .....	104
The Stability Function .....	108
Construction of Methods of Order 4 .....	108
Higher Order Methods .....	111
Implementation of Rosenbrock-Type Methods .....	111
The “Hump” .....	113
Methods with Inexact Jacobian ( $W$ -Methods) .....	114
Exercises .....	117
<b>IV.8 Implementation of Implicit Runge-Kutta Methods</b> .....	118
Reformulation of the Nonlinear System .....	118
Simplified Newton Iterations .....	119
The Linear System .....	121
Step Size Selection .....	123
Implicit Differential Equations .....	127
An SDIRK-Code .....	128
SIRK-Methods .....	128
Exercises .....	130
<b>IV.9 Extrapolation Methods</b> .....	131
Extrapolation of Symmetric Methods .....	131
Smoothing .....	133
The Linearly Implicit Mid-Point Rule .....	134
Implicit and Linearly Implicit Euler Method .....	138
Implementation .....	139
Exercises .....	142
<b>IV.10 Numerical Experiments</b> .....	143
The Codes Used .....	143
Twelve Test Problems .....	144
Results and Discussion .....	152
Partitioning and Projection Methods .....	160
Exercises .....	165
<b>IV.11 Contractivity for Linear Problems</b> .....	167
Euclidean Norms (Theorem of von Neumann) .....	168
Error Growth Function for Linear Problems .....	169
Small Nonlinear Perturbations .....	172
Contractivity in $\ \cdot\ _\infty$ and $\ \cdot\ _1$ .....	175
Study of the Threshold Factor .....	176

	Absolutely Monotonic Functions .....	178
	Exercises .....	179
<b>IV.12</b>	<b>B-Stability and Contractivity</b> .....	180
	One-Sided Lipschitz Condition .....	180
	$B$ -Stability and Algebraic Stability .....	181
	Some Algebraically Stable IRK Methods .....	183
	$AN$ -Stability .....	184
	Reducible Runge-Kutta Methods .....	187
	The Equivalence Theorem for $S$ -Irreducible Methods .....	188
	Error Growth Function .....	193
	Computation of $\varphi_B(x)$ .....	195
	Exercises .....	199
<b>IV.13</b>	<b>Positive Quadrature Formulas and B-Stable RK-Methods</b> ..	201
	Quadrature Formulas and Related Continued Fractions .....	201
	Number of Positive Weights .....	203
	Characterization of Positive Quadrature Formulas .....	205
	Necessary Conditions for Algebraic Stability .....	206
	Characterization of Algebraically Stable Methods .....	209
	The “Equivalence” of $A$ - and $B$ -Stability .....	211
	Exercises .....	213
<b>IV.14</b>	<b>Existence and Uniqueness of IRK Solutions</b> .....	215
	Existence .....	215
	A Counterexample .....	217
	Influence of Perturbations and Uniqueness .....	218
	Computation of $\alpha_0(A^{-1})$ .....	220
	Methods with Singular $A$ .....	222
	Lobatto IIIC Methods .....	223
	Exercises .....	223
<b>IV.15</b>	<b>B-Convergence</b> .....	225
	The Order Reduction Phenomenon .....	225
	The Local Error .....	228
	Error Propagation .....	229
	$B$ -Convergence for Variable Step Sizes .....	230
	$B$ -Convergence Implies Algebraic Stability .....	232
	The Trapezoidal Rule .....	234
	Order Reduction for Rosenbrock Methods .....	236
	Exercises .....	237

## Chapter V. Multistep Methods for Stiff Problems

<b>V.1</b>	<b>Stability of Multistep Methods</b> .....	240
	The Stability Region .....	240
	Adams Methods .....	242
	Predictor-Corrector Schemes .....	244
	Nyström Methods .....	245
	BDF .....	246
	The Second Dahlquist Barrier .....	247
	Exercises .....	249
<b>V.2</b>	<b>“Nearly” A-Stable Multistep Methods</b> .....	250
	$A(\alpha)$ -Stability and Stiff Stability .....	250
	High Order $A(\alpha)$ -Stable Methods .....	251
	Approximating Low Order Methods with High Order Ones .....	253

	A Disc Theorem .....	254
	Accuracy Barriers for Linear Multistep Methods .....	254
	Exercises .....	259
<b>V.3</b>	<b>Generalized Multistep Methods</b> .....	261
	Second Derivative Multistep Methods of Enright .....	261
	Second Derivative BDF Methods .....	265
	Blended Multistep Methods .....	266
	Extended Multistep Methods of Cash .....	267
	Multistep Collocation Methods .....	270
	Methods of “Radau” Type .....	273
	Exercises .....	275
<b>V.4</b>	<b>Order Stars on Riemann Surfaces</b> .....	279
	Riemann Surfaces .....	279
	Poles Representing Numerical Work .....	283
	Order and Order Stars .....	284
	The “Daniel and Moore Conjecture” .....	286
	Methods with Property $C$ .....	288
	General Linear Methods .....	290
	Dual Order Stars .....	295
	Exercises .....	297
<b>V.5</b>	<b>Experiments with Multistep Codes</b> .....	300
	The Codes Used .....	300
	Exercises .....	304
<b>V.6</b>	<b>One-Leg Methods and <math>G</math>-Stability</b> .....	305
	One-Leg (Multistep) Methods .....	305
	Existence and Uniqueness .....	306
	$G$ -Stability .....	307
	An Algebraic Criterion .....	309
	The Equivalence of $A$ -Stability and $G$ -Stability .....	310
	A Criterion for Positive Functions .....	313
	Error Bounds for One-Leg Methods .....	314
	Convergence of $A$ -Stable Multistep Methods .....	317
	Exercises .....	319
<b>V.7</b>	<b>Convergence for Linear Problems</b> .....	321
	Difference Equations for the Global Error .....	321
	The Kreiss Matrix Theorem .....	323
	Some Applications of the Kreiss Matrix Theorem .....	326
	Global Error for Prothero and Robinson Problem .....	328
	Convergence for Linear Systems with Constant Coefficients .....	329
	Matrix Valued Theorem of von Neumann .....	330
	Discrete Variation of Constants Formula .....	332
	Exercises .....	337
<b>V.8</b>	<b>Convergence for Nonlinear Problems</b> .....	339
	Problems Satisfying a One-Sided Lipschitz Condition .....	339
	Multiplier Technique .....	342
	Multipliers and Nonlinearities .....	346
	Discrete Variation of Constants and Perturbations .....	348
	Convergence for Nonlinear Parabolic Problems .....	349
	Exercises .....	354
<b>V.9</b>	<b>Algebraic Stability of General Linear Methods</b> .....	356
	$G$ -Stability .....	356

Algebraic Stability .....	357
$AN$ -Stability and Equivalence Results .....	359
Multistep Runge-Kutta Methods .....	362
Simplifying Assumptions .....	363
Quadrature Formulas .....	365
Algebraically Stable Methods of Order $2s$ .....	366
$B$ -Convergence .....	368
Exercises .....	370

## Chapter VI. Singular Perturbation Problems and Index 1 Problems

<b>VI.1 Solving Index 1 Problems</b> .....	372
Asymptotic Solution of van der Pol's Equation .....	372
The $\epsilon$ -Embedding Method for Problems of Index 1 .....	374
State Space Form Method .....	375
A Transistor Amplifier .....	376
Problems of the Form $Mu' = \varphi(u)$ .....	378
Convergence of Runge-Kutta Methods .....	380
Exercises .....	381
<b>VI.2 Multistep Methods</b> .....	382
Methods for Index 1 Problems .....	382
Convergence for Singular Perturbation Problems .....	383
Exercises .....	387
<b>VI.3 Epsilon Expansions for Exact and RK Solutions</b> .....	388
Expansion of the Smooth Solution .....	388
Expansions with Boundary Layer Terms .....	389
Estimation of the Remainder .....	391
Expansion of the Runge-Kutta Solution .....	392
Convergence of RK-Methods for Differential-Algebraic Systems .....	394
Existence and Uniqueness of the Runge-Kutta Solution .....	397
Influence of Perturbations .....	398
Estimation of the Remainder in the Numerical Solution .....	399
Numerical Confirmation .....	403
Perturbed Initial Values .....	405
Exercises .....	406
<b>VI.4 Rosenbrock Methods</b> .....	407
Definition of the Method .....	407
Derivatives of the Exact Solution .....	408
Trees and Elementary Differentials .....	409
Taylor Expansion of the Exact Solution .....	411
Taylor Expansion of the Numerical Solution .....	412
Order Conditions .....	415
Convergence .....	416
Stiffly Accurate Rosenbrock Methods .....	418
Construction of RODAS, a Stiffly Accurate Embedded Method .....	420
Inconsistent Initial Values .....	422
Exercises .....	424
<b>VI.5 Extrapolation Methods</b> .....	426
Linearly Implicit Euler Discretization .....	426
Perturbed Asymptotic Expansion .....	428
Order Tableau .....	431

Error Expansion for Singular Perturbation Problems	433
Dense Output	438
Exercises	441
<b>VI.6 Quasilinear Problems</b>	442
Example: Moving Finite Elements	442
Problems of Index One	445
Numerical Treatment of $C(y)y' = f(y)$	446
Extrapolation Methods	447
Exercises	448

## Chapter VII. Differential-Algebraic Equations of Higher Index

<b>VII.1 The Index and Various Examples</b>	452
Linear Equations with Constant Coefficients	452
Differentiation Index	454
Differential Equations on Manifolds	457
The Perturbation Index	459
Control Problems	461
Mechanical Systems	463
Exercises	465
<b>VII.2 Index Reduction Methods</b>	468
Index Reduction by Differentiation	468
Stabilization by Projection	470
Differential Equations with Invariants	472
Methods Based on Local State Space Forms	474
Overdetermined Differential-Algebraic Equations	477
Unstructured Higher Index Problems	478
Exercises	480
<b>VII.3 Multistep Methods for Index 2 DAE</b>	481
Existence and Uniqueness of Numerical Solution	482
Influence of Perturbations	484
The Local Error	485
Convergence for BDF	486
General Multistep Methods	489
Solution of the Nonlinear System by Simplified Newton	490
Exercises	491
<b>VII.4 Runge-Kutta Methods for Index 2 DAE</b>	492
The Nonlinear System	492
Estimation of the Local Error	494
Convergence for the $y$ -Component	496
Convergence for the $z$ -Component	497
Collocation Methods	498
Superconvergence of Collocation Methods	500
Projected Runge-Kutta Methods	502
Summary of Convergence Results	504
Exercises	505
<b>VII.5 Order Conditions for Index 2 DAE</b>	506
Derivatives of the Exact Solution	506
Trees and Elementary Differentials	507
Taylor Expansion of the Exact Solution	508

Derivatives of the Numerical Solution .....	510
Order Conditions .....	512
Simplifying Assumptions .....	514
Projected Runge-Kutta Methods .....	515
Exercises .....	518
<b>VII.6 Half-Explicit Methods for Index 2 Systems .....</b>	<b>519</b>
Half-Explicit Runge-Kutta Methods .....	520
Extrapolation Methods .....	525
$\beta$ -Blocked Multistep Methods .....	527
Exercises .....	529
<b>VII.7 Computation of Multibody Mechanisms .....</b>	<b>530</b>
Description of the Model .....	530
Fortran Subroutines .....	533
Computation of Consistent Initial Values .....	535
Numerical Computations .....	536
A Stiff Mechanical System .....	541
Exercises .....	542
<b>VII.8 Symplectic Methods for Constrained Hamiltonian Systems ..</b>	<b>543</b>
Properties of the Exact Flow .....	544
First Order Symplectic Method .....	545
SHAKE and RATTLE .....	548
The Lobatto IIIA-III B Pair .....	550
Composition Methods .....	554
Backward Error Analysis (for ODEs) .....	555
Backward Error Analysis on Manifolds .....	559
Exercises .....	562
<b>Appendix. Fortran Codes .....</b>	<b>565</b>
Driver for the Code RADAU5 .....	566
Subroutine RADAU5 .....	568
Subroutine RADAUP .....	574
Subroutine RODAS .....	574
Subroutine SEULEX .....	575
Problems with Special Structure .....	575
Use of SOLOUT and of Dense Output .....	576
<b>Bibliography .....</b>	<b>577</b>
<b>Symbol Index .....</b>	<b>605</b>
<b>Subject Index .....</b>	<b>607</b>