

# 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 .....	5
	Diffusion .....	5
	A “Stiff” Beam .....	9
	High Oscillations .....	12
	Exercises .....	12
<b>IV.2</b>	<b>Stability Analysis for Explicit RK Methods</b> .....	16
	Stability Analysis for Euler’s Method .....	16
	Explicit RK Methods .....	17
	Extrapolation Methods .....	19
	Analysis of the Examples of IV.1 .....	20
	Automatic Stiffness Detection .....	22
	Step-Control Stability .....	26
	<i>SC</i> -Stable Dormand and Prince Pairs .....	28
	A PI Step Size Control .....	31
	Exercises .....	36
<b>IV.3</b>	<b>A-Stable Runge-Kutta Methods</b> .....	40
	The Stability Function .....	40
	A-Stability .....	42
	L-Stability .....	45
	A( $\alpha$ )-Stability .....	46
	Numerical Results .....	47
	Collocation Methods .....	48
	Padé Approximations to the Exponential Function .....	50
	Exercises .....	51
<b>IV.4</b>	<b>Order Stars</b> .....	53
	Introduction .....	53
	Order and Stability for Rational Approximations .....	58
	Stability of Padé Approximations .....	60
	Comparing Stability Domains .....	61
	Rational Approximations with Real Poles .....	64
	The Real-Pole Sandwich .....	65
	Multiple Real-Pole Approximations .....	70
	Exercises .....	72

<b>IV.5 Construction of Implicit Runge-Kutta Methods</b> .....	75
Gauss Methods .....	75
Radau IA and Radau IIA Methods .....	76
Lobatto IIIA, IIIB and IIIC Methods .....	79
The $W$ -Transformation .....	82
Construction of Implicit Runge-Kutta Methods .....	88
Stability Function .....	89
Positive Functions .....	91
Exercises .....	94
<b>IV.6 Diagonally Implicit RK Methods</b> .....	97
Order Conditions .....	97
Stiffly Accurate SDIRK Methods .....	99
Solution of Equations (6.4) .....	101
The Stability Function .....	103
Multiple Real-Pole Approximations with $R(\infty) = 0$ .....	105
Choice of Method .....	106
Exercises .....	108
<b>IV.7 Rosenbrock-Type Methods</b> .....	110
Derivation of the Method .....	110
Order Conditions .....	112
The Stability Function .....	116
Construction of Methods of Order 4 .....	117
Higher Order Methods .....	119
Implementation of Rosenbrock-Type Methods .....	120
Coding .....	121
The "Hump" .....	122
Methods with Inexact Jacobian ( $W$ -Methods) .....	123
Exercises .....	126
<b>IV.8 Implementation of Implicit Runge-Kutta Methods</b> .....	128
Reformulation of the Nonlinear System .....	128
Simplified Newton Iterations .....	129
Stopping Criterion .....	130
The Linear System .....	131
Transformation to Hessenberg Form .....	132
Starting Values for the Newton Iteration .....	133
Step Size Selection .....	133
Numerical Study of the Step-Control Mechanism .....	135
Implicit Differential Equations .....	136
Banded Jacobian .....	138
An SDIRK-Code .....	138
SIRK-Methods .....	139
Exercises .....	140
<b>IV.9 Extrapolation Methods</b> .....	142
Extrapolation of Symmetric Methods .....	142
Smoothing .....	144
The Linearly Implicit Mid-Point Rule .....	145
Implicit and Linearly Implicit Euler Method .....	150
Implementation .....	151
Non-Autonomous Differential Equations .....	153
Implicit Differential Equations .....	153
Exercises .....	154

<b>IV.10 Numerical Experiments</b> .....	155
The Codes Used .....	155
Small Test Problems .....	156
Large Test Problems .....	159
Results and Discussion .....	165
Possible Improvements .....	169
Partitioning and Projection Methods .....	171
The Method of Gear and Saad .....	172
The EKBWH-Method .....	174
Exercises .....	176
<b>IV.11 Contractivity for Linear Problems</b> .....	178
Euclidean Norms (Theorem of von Neumann) .....	179
Study of the Contractivity Function .....	180
Small Nonlinear Perturbations .....	182
Contractivity in $\ \cdot\ _\infty$ and $\ \cdot\ _1$ .....	185
Study of the Threshold Factor .....	187
Absolutely Monotonic Functions .....	188
Exercises .....	190
<b>IV.12 <i>B</i>-Stability and Contractivity</b> .....	191
One-Sided Lipschitz Condition .....	191
<i>B</i> -Stability .....	192
Algebraic Stability .....	193
Some Algebraically Stable IRK Methods .....	194
<i>AN</i> -Stability .....	196
Reducible Runge-Kutta Methods .....	199
The Equivalence Theorem for <i>S</i> -Irreducible Methods .....	201
( <i>k, l</i> )-Algebraic Stability .....	206
Computation of the Optimal <i>k</i> .....	207
Exercises .....	211
<b>IV.13 Positive Quadrature Formulas and <i>B</i>-Stable RK Methods</b> ..	214
Quadrature Formulas and Related Continued Fractions .....	214
Number of Positive Weights .....	217
Characterization of Positive Quadrature Formulas .....	219
Necessary Conditions for Algebraic Stability .....	220
Characterization of Algebraically Stable Methods .....	223
The "Equivalence" of <i>A</i> - and <i>B</i> -Stability .....	225
Exercises .....	227
<b>IV.14 Existence and Uniqueness of IRK Solutions</b> .....	229
Existence .....	229
A Counterexample .....	231
Influence of Perturbations and Uniqueness .....	233
Computation of $\alpha_0(A^{-1})$ .....	234
Methods with Singular <i>A</i> .....	236
Lobatto IIC Methods .....	238
Exercises .....	238
<b>IV.15 <i>B</i>-Convergence</b> .....	240
The Order Reduction Phenomenon .....	240
The Local Error .....	243
Error Propagation .....	245
<i>B</i> -Convergence for Variable Step Sizes .....	246

<i>B</i> -Convergence Implies Algebraic Stability .....	247
The Trapezoidal Rule .....	250
Order Reduction for Rosenbrock Methods .....	252
Exercises .....	253

## Chapter V. Multistep Methods for Stiff Problems

<b>V.1 Stability of Multistep Methods</b> .....	256
The Stability Region .....	256
Computation of the Stability Domain .....	257
Adams Methods .....	259
Predictor-Corrector Schemes .....	260
Nyström Methods .....	262
BDF .....	263
<i>A</i> -stability and the Second Dahlquist Barrier .....	264
Exercises .....	266
<b>V.2 “Nearly” <i>A</i>-Stable Multistep Methods</b> .....	268
<i>A</i> ( $\alpha$ )-Stability and Stiff Stability .....	268
High Order <i>A</i> ( $\alpha$ )-Stable Methods .....	269
Approximating Low Order Methods with High Order Ones .....	271
A Disc Theorem .....	272
Accuracy Barriers for Linear Multistep Methods .....	273
Exercises .....	277
<b>V.3 Generalized Multistep Methods</b> .....	280
Second Derivative Multistep Methods .....	280
Dense Output for Enright Methods .....	282
Second Derivative BDF Methods .....	284
Blended Multistep Methods .....	285
Extended Multistep Methods .....	287
Multistep Collocation Methods .....	290
Methods of “Radau” Type .....	293
Computation of the Nodes .....	294
Stability of the Radau-Type Methods .....	295
Exercises .....	296
<b>V.4 Order Stars on Riemann Surfaces</b> .....	300
Riemann Surfaces .....	300
More General Methods .....	303
Poles Representing Numerical Work .....	305
Order and Order Stars .....	306
The “Daniel and Moore Conjecture” .....	308
Methods with Property <i>C</i> .....	311
General Linear Methods .....	313
Dual Order Stars .....	318
Exercises .....	320
<b>V.5 Experiments with Multistep Codes</b> .....	323
The Codes Used .....	323
<b>V.6 One-Leg Methods and <i>G</i>-Stability</b> .....	329
One-Leg (Multistep) Methods .....	329
Existence and Uniqueness .....	331
<i>G</i> -Stability .....	332

	An Algebraic Criterion .....	333
	The Equivalence of $A$ -Stability and $G$ -Stability .....	334
	A Criterion for Positive Functions .....	337
	Error Bounds for One-Leg Methods .....	338
	Convergence of $A$ -Stable Multistep Methods .....	342
	Exercises .....	344
<b>V.7</b>	<b>Convergence for Linear Problems</b> .....	346
	Difference Equations for the Global Error .....	346
	Formulation as a One-Step Method .....	348
	The Kreiss Matrix Theorem .....	348
	Some Applications of the Kreiss Matrix Theorem .....	351
	Global Error for Prothero and Robinson Problem .....	353
	Convergence for Linear Systems with Constant Coefficients .....	354
	Matrix Valued Theorem of von Neumann .....	356
	Discrete Variation of Constants Formula .....	357
	Exercises .....	363
<b>V.8</b>	<b>Convergence for Nonlinear Problems</b> .....	365
	Problems Satisfying a One-Sided Lipschitz Condition .....	365
	Multiplier Technique .....	368
	Construction of Multipliers .....	371
	Multipliers and Nonlinearities .....	373
	Discrete Variation of Constants and Perturbations .....	374
	Incompressible Navier-Stokes Equations .....	376
	Convergence for Nonlinear Parabolic Problems .....	378
	Exercises .....	381
<b>V.9</b>	<b>Algebraic Stability of General Linear Methods</b> .....	383
	$G$ -Stability .....	383
	Algebraic Stability .....	384
	$AN$ -Stability and Equivalence Results .....	387
	Multistep Runge-Kutta Methods .....	390
	Simplifying Assumptions .....	391
	Quadrature Formulas .....	393
	Algebraically Stable Methods of Order $2s$ .....	394
	$B$ -Convergence .....	396
	Exercises .....	398

## Chapter VI. Singular Perturbation Problems and Differential-Algebraic Equations

<b>VI.1</b>	<b>Singular Perturbation and Index 1 Problems</b> .....	400
	Asymptotic Solution of van der Pol's Equation .....	400
	Runge-Kutta Methods for Problems of Index 1 .....	402
	A Transistor Amplifier .....	404
	Problems of the Form $Mu' = \varphi(u)$ .....	406
	Convergence of Runge-Kutta Methods .....	408
	Multistep Methods for Index 1 DAE's .....	410
	Multistep Methods for Singular Perturbation Problems .....	411
	Exercises .....	415
<b>VI.2</b>	<b>Epsilon Expansions for Exact and RK Solutions</b> .....	416
	Expansion of the Smooth Solution .....	416

	Expansions with Boundary Layer Terms .....	417
	Estimation of the Remainder .....	420
	Expansion of the Runge-Kutta Solution .....	421
	Convergence of RK-Methods for Differential-Algebraic Systems .....	423
	Existence and Uniqueness of the Runge-Kutta Solution .....	425
	Influence of Perturbations .....	426
	Estimation of the Remainder in the Numerical Solution .....	428
	Numerical Confirmation .....	432
	Perturbed Initial Values .....	432
	Exercises .....	435
<b>VI.3</b>	<b>Rosenbrock Methods</b> .....	436
	Definition of the Method .....	436
	Derivatives of the Exact Solution .....	438
	Trees and Elementary Differentials .....	438
	Taylor Expansion of the Exact Solution .....	440
	Taylor Expansion of the Numerical Solution .....	442
	Order Conditions .....	445
	Convergence .....	447
	Stiffly Accurate Rosenbrock Methods .....	448
	Construction of RODAS, a Stiffly Accurate Embedded Method.....	450
	Inconsistent Initial Values .....	453
	Exercises .....	455
<b>VI.4</b>	<b>Extrapolation Methods</b> .....	457
	Linearly Implicit Euler Discretization .....	457
	Perturbed Asymptotic Expansion .....	460
	Order Tableau .....	463
	Error Expansion for Singular Perturbation Problems .....	465
	Dense Output .....	470
	Exercises .....	473
<b>VI.5</b>	<b>Higher Index Problems</b> .....	474
	The Weierstrass–Kronecker Canonical Form .....	474
	The Differential Index .....	476
	The Perturbation Index .....	478
	Control Problems .....	481
	Mechanical Systems .....	483
	Problems of the Form $M(u)u' = \varphi(u)$ .....	486
	Exercises .....	487
<b>VI.6</b>	<b>Multistep Methods for Index 2 DAE</b> .....	489
	Existence and Uniqueness of Numerical Solution .....	490
	Influence of Perturbations .....	492
	The Local Error .....	494
	Convergence for BDF .....	494
	General Multistep Methods .....	498
	Solution of the Nonlinear System by Simplified Newton .....	499
	Exercises .....	500
<b>VI.7</b>	<b>Runge-Kutta Methods for Index 2 DAE</b> .....	502
	The Nonlinear System .....	502
	Estimation of the Local Error .....	504
	Convergence for the $y$ -Component .....	506
	Convergence for the $z$ -Component .....	508

Collocation Methods .....	508
Superconvergence of Collocation Methods .....	510
Projected Runge-Kutta Methods .....	512
Summary of Convergence Results .....	514
Exercises .....	515
<b>VI.8 Order Conditions for Index 2 DAE .....</b>	<b>517</b>
Derivatives of the Exact Solution .....	517
Trees and Elementary Differentials .....	518
Taylor Expansion of the Exact Solution .....	520
Derivatives of the Numerical Solution .....	521
Order Conditions .....	524
Simplifying Assumptions .....	525
Projected Runge-Kutta Methods .....	527
Exercises .....	530
<b>VI.9 Computation of Multibody Mechanisms .....</b>	<b>531</b>
Description of the Model .....	531
Fortran Subroutines .....	536
Computation of Consistent Initial Values .....	538
Numerical Computations .....	539
A Stiff Mechanical System .....	544
Exercises .....	545
<b>Appendix Fortran Codes .....</b>	<b>547</b>
Driver for the Code RADAU5 .....	547
Subroutine RADAU5 .....	550
Subroutine SDIRK4 .....	555
Subroutine ROS4 .....	557
Subroutine RODAS .....	558
Subroutine SEULEX .....	560
Subroutine SODEX .....	562
<b>Bibliography .....</b>	<b>565</b>
<b>Symbol Index .....</b>	<b>593</b>
<b>Subject Index .....</b>	<b>595</b>