

E. Hairer

S. P. Norsett

G. Wanner

# **Solving Ordinary Differential Equations I**

#### **Nonstiff Problems**

Second Revised Edition With 135 Figures



## Contents

## Chapter I. Classical Mathematical Theory

1.1	Terminology	2
1.2	The Oldest Differential Equations  Newton	4
	Leibniz and the Bernoulli Brothers.  Variational Calculus.  Clairaut.  Exercises.	7
1.3	Elementary Integration Methods.  First Order Equations. Second Order Equations. Exercises.	12 13
1.4	Linear Differential Equations  Equations with Constant Coefficients.  Variation of Constants.  Exercises.	16 18
1.5	Equations with Weak Singularities. Linear Equations. Nonlinear Equations. Exercises.	20
1.6	Systems of Equations The Vibrating String and Propagation of Sound. Fourier Lagrangian Mechanics. Hamiltonian Mechanics. Exercises	26 29 30 32
1.7	A General Existence Theorem  Convergence of Euler's Method  Existence Theorem of Peano.  Exercises.	35 41
1.8	Existence Theory using Iteration Methods and Taylor Series Picard-Lindelof Iteration. Taylor Scries. Recursive Computation of Taylor Coefficients. I • xcrciscs.	45 46 47

#### Contents

1.9	Vector Notation.	. 51
	Subordinate Matrix Norms.	52 53
	Exercises.	
1.10	Differential Inequalities	
1.10	Introduction	
	The Fundamental Theorems.	57
	Estimates Using One-Sided Lipschitz Conditions.	
	Exercises	
1.11	Systems of Linear Differential Equations	
1.11	Resolvent and Wronskian.	65
	Inhomogeneous Linear Equations.	66
	The Abel-Liouville-Jacobi-Ostrogradskii Identity.	66
	Exercises	
1.12	Systems with Constant Coefficients	69
	Linearization	
	Diagonalization	
	The Schur Decomposition.	70
	Numerical Computations	
	The Jordan Canonical Form	
	Geometric Representation	
	Exercises.	
1.13	Stability	
	Introduction	80
	The Routh-Hurwitz Criterion	81
	Computational Considerations.	85
	Liapunov Functions.	86
	Stability of Nonlinear Systems	
	Exercises	
1.14	Derivatives with Respect to Parameters and Initial Values	92
	The Derivative with Respect to a Parameter	95
	The Nonlinear Variation-of-Constants Formula.	
	Flows and Volume-Preserving Flows.	97
	Canonical Equations and Symplectic Mappings.	100
	Exercises	104
1.15	Boundary Value and Eigenvalue Problems	
1.15	Boundary Value Problems.	105
	Sturm-Liouville Eigenvalue Problems	107
	Exercises	
1.16	Periodic Solutions, Limit Cycles, Strange Attractors	
1.10	Van der Pol's Equation	. III
	Chemical Reactions.	115
	Limit Cycles in Higher Dimensions, Hopf Bifurcation.	117
	Strange Attractors.	
	The Ups and Downs of the Lorenz Model	. 123
	Feigenbaum Cascades	. 124
	Exercises	126

Cna	ipter 11. Runge-Kutta and Extrapolation Me	etnoas
11.1	The First Runge-Kutta Methods.  General Formulation of Runge-Kutta Methods.  Discussion of Methods of Order 4.  "Optimal" Formulas.  Numerical Example.  Exercises.	134 135 139 140
11.2	Order Conditions for Runge-Kutta Methods. The Derivatives of the True Solution. Conditions for Order 3. Trees and Elementary Differentials. The Taylor Expansion of the True Solution. Faa di Bruno's Formula. The Derivatives of the Numerical Solution. The Order Conditions. Exercises.	
11.3	Error Estimation and Convergence for RK Methods.  Rigorous Error Bounds.  The Principal Error Term.  Estimation of the Global Error.  Exercises.	156 158 159
11.4	Practical Error Estimation and Step Size Selection. Richardson Extrapolation. Embedded Runge-Kutta Formulas. Automatic Step Size Control. Starting Step Size. Numerical Experiments. Exercises.	164 165 167 169 170
11.5	Explicit Runge-Kutta Methods of Higher Order. The Butcher Barriers. 6-Stage, 5th Order Processes. Embedded Formulas of Order 5. Higher Order Processes. Embedded Formulas of High Order. An 8th Order Embedded Method. Exercises.	173 175 176 180 181
11.6	Dense Output, Discontinuities, Derivatives  Dense Output.  Continuous Dormand & Prince Pairs.  Dense Output for DOP853.  Event Location.  Discontinuous Equations.  Numerical Computation of Derivatives with Respect to Initial Values and Parameters.  Exercises.	
11.7	Implicit Runge-Kutta Methods.  Existence of a Numerical Solution.  The Methods of Kuntzmann and Butcher of Order 2s.  IRK Methods Based on Lobatto Quadrature.	204 206 208

#### XII Contents

	Collocation Methods.  Exercises.	
11.8	Asymptotic Expansion of the Global Error.  The Global Error.	216
	Variable h	
	Negative h	
	Properties of the Adjoint Method.	
	Symmetric Methods	
	Exercises	
11.9	Extrapolation Methods	224
	Definition of the Method	
	The Aitken - Neville Algorithm.	
	The Gragg or GBS Method	
	Asymptotic Expansion for Odd Indices	231
	Existence of Explicit RK Methods of Arbitrary Order.	
	Order and Step Size Control.	233
	Dense Output for the GBS Method	
	Control of the Interpolation Error	
11 10		
11.10	Numerical Comparisons	244
	Problems.  Performance of the Codes.	244
	A "Stretched" Error Estimator for DOP853.	254
	Effect of Step-Number Sequence in ODEX.	
11.11	Parallel Methods	
11,11	Parallel Runge-Kutta Methods.	258
	Parallel Iterated Runge-Kutta Methods.	259
	Extrapolation Methods	
	Increasing Reliability	261
	Exercises	
11.12	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".	
	Exercises	
11.13	Higher Derivative Methods.	
	Collocation Methods.	
	Hermite-Obreschkoff Methods	
	Fehlberg Methods.	
	General Theory of Order Conditions	
11 14		
11.14	Numerical Methods for Second Order Differential Equations Nystrom Methods.	
	The Derivatives of the Exact Solution.	286
	The Derivatives of the Numerical Solution.	288
	The Order Conditions.	
	On the Construction of Nystrdm Methods.	
	An Extrapolation Method for $y'' = f(x, y)$	294
	Problems for Numerical Comparisons.	296

	Contents	XIII
	Performance of the Codes	
11.15	P-Series for Partitioned Differential Equations.  Derivatives of the Exact Solution, P-Trees.  P-Series.  Order Conditions for Partitioned Runge-Kutta Methods.	303 306 307
	Further Applications of P-Series	
11.16	Symplectic Runge-Kutta Methods.	315
	An Example from Galactic Dynamics.  Partitioned Runge-Kutta Methods.  Symplectic Nystrom Methods.	326 330
	Conservation of the Hamiltonian; Backward Analysis Exercises	
11.17	<b>Delay Differential Equations</b> Existence	339
	Constant Step Size Methods for Constant Delay.  Variable Step Size Methods.  Stability.	342
	An Example from Population Dynamics.  Infectious Disease Modelling.	345
	An Example from Enzyme Kinetics	248 349
	Integro-Differential Equations Exercises	
	pter III. Multistep Methods General Linear Methods	
111.1	Classical Linear Multistep Formulas	
	Explicit Adams Methods	
	Numerical Experiment	361
	Explicit Nystrom Methods.	
	Milne-Simpson Methods	363 364
	Exercises.	
111.2	Local Error and Order Conditions	
	Local Error of a Multistep Method	
	Order of a Multistep Method	
	Irreducible Methods.	
	The Peano Kernel of a Multistep Method	
	Exercises	377
HL3	Stability and the First Dahlquist Barrier	
	Stability of the BDF-Formulas	
	Highest Attainable Order of Stable Multistep Methods Exercises	

111.4	Convergence of Multistep Methods	
	Formulation as One-Step Method.	393
	Proof of Convergence.	. 395
	Exercises	. 396
111.5	Variable Step Size Multistep Methods	397
	Variable Step Size Adams Methods.	
	Recurrence Relations for $gj(n)$ , $\$j(n)$ and $\$j(n)$ .	399
	Variable Step Size BDF	400
	General Variable Step Size Methods and Their Orders	401
	Stability	402
	Convergence	
	Exercises	409
111.6	Nordsieck Methods	410
	Equivalence with Multistep Methods.	412
	Implicit Adams Methods	417
	BDF-Methods.	
	Exercises	
111.7	Implementation and Numerical Comparisons	
	Step Size and Order Selection	
	Some Available Codes	
	Numerical Comparisons.	427
111.8	General Linear Methods	
111.0	A General Integration Procedure.	431
	Stability and Order.	
	Convergence.	
	Order Conditions for General Linear Methods.	441
	Construction of General Linear Methods.	
	Exercises.	
111.9	Asymptotic Expansion of the Global Error	
1110	An Instructive Example.	
	Asymptotic Expansion for Strictly Stable Methods (8.4).	450
	Weakly Stable Methods.	454
	The Adjoint Method	
	Symmetric Methods	459
	Exercises	
111.10	Multistep Methods for Second Order Differential Equations	
11111	Explicit Stormer Methods	462
	Implicit Stormer Methods.	464
	Numerical Example	
	General Formulation.	
	Convergence	468
	Asymptotic Formula for the Global Error	471
	Rounding Errors	
	Exercises	
Appe	endix. Fortran Codes	475
	Driver for the Code DOPRI5.	475
	Subroutine D0PRI5.	
	Subroutine DOP853	
	Subroutine ODEX	482

	Contents	XV
Subroutine 0DEX2.  Driver for the Code RETARD.  Subroutine RETARD.		486
Bibliography		491
Symbol Index		521
Subject Index		523