



**UNIVERSITÉ
DE GENÈVE**

Archive ouverte UNIGE

<https://archive-ouverte.unige.ch>

Livre

1993

Extract

Open Access

This file is a(n) Extract of:

Solving Ordinary Differential Equations I. Nonstiff Problems

Hairer, Ernst; Norsett, Syvert Paul; Wanner, Gerhard

This publication URL:

<https://archive-ouverte.unige.ch/unige:12346>

Publication DOI:

[10.1007/978-3-540-78862-1](https://doi.org/10.1007/978-3-540-78862-1)

© This document is protected by copyright. Please refer to copyright holders for terms of use.

**Springer Series in
Computational
Mathematics**

8

Editorial Board

R. Bank

R.L. Graham

J. Stoer

R. Varga

H. Yserentant

E. Hairer
S. P. Nørsett
G. Wanner

Solving Ordinary Differential Equations I

Nonstiff Problems

Second Revised Edition
With 135 Figures

 Springer

Ernst Hairer
Gerhard Wanner
Université de Genève
Section de Mathématiques
2–4 rue du Lièvre
1211 Genève 4
Switzerland
Ernst.Hairer@math.unige.ch
Gerhard.Wanner@math.unige.ch

Syvrt P. Nørsett
Norwegian University of Science
and Technology (NTNU)
Department of Mathematical Sciences
7491 Trondheim
Norway
norsett@math.ntnu.no

Corrected 3rd printing 2008

ISBN 978-3-540-56670-0

e-ISBN 978-3-540-78862-1

DOI 10.1007/978-3-540-78862-1

Springer Series in Computational Mathematics ISSN 0179-3632

Library of Congress Control Number: 93007847

Mathematics Subject Classification (2000): 65Lxx, 34A50

© 1993, 1987 Springer-Verlag Berlin Heidelberg

This work is subject to copyright. All rights are reserved, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilm or in any other way, and storage in data banks. Duplication of this publication or parts thereof is permitted only under the provisions of the German Copyright Law of September 9, 1965, in its current version, and permission for use must always be obtained from Springer. Violations are liable to prosecution under the German Copyright Law.

The use of general descriptive names, registered names, trademarks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

Cover design: WMX Design GmbH, Heidelberg

Typesetting: by the authors

Production: LE-TeX Jelonek, Schmidt & Vöckler GbR, Leipzig

Printed on acid-free paper

9 8 7 6 5 4 3 2 1

springer.com

This edition is dedicated to
Professor John Butcher
on the occasion of his 60th birthday

His unforgettable lectures on Runge-Kutta methods, given in June 1970 at the University of Innsbruck, introduced us to this subject which, since then, we have never ceased to love and to develop with all our humble abilities.

From the Preface to the First Edition

So far as I remember, I have never seen an Author's Preface which had any purpose but one — to furnish reasons for the publication of the Book. (Mark Twain)

Gauss' dictum, "when a building is completed no one should be able to see any trace of the scaffolding," is often used by mathematicians as an excuse for neglecting the motivation behind their own work and the history of their field. Fortunately, the opposite sentiment is gaining strength, and numerous asides in this Essay show to which side go my sympathies. (B.B. Mandelbrot 1982)

This gives us a good occasion to work out most of the book until the next year. (the Authors in a letter, dated Oct. 29, 1980, to Springer-Verlag)

There are two volumes, one on non-stiff equations, . . . , the second on stiff equations, The first volume has three chapters, one on classical mathematical theory, one on Runge-Kutta and extrapolation methods, and one on multistep methods. There is an Appendix containing some Fortran codes which we have written for our numerical examples.

Each chapter is divided into sections. Numbers of formulas, theorems, tables and figures are consecutive in each section and indicate, in addition, the section number, but not the chapter number. Cross references to other chapters are rare and are stated explicitly. . . . References to the Bibliography are by "Author" plus "year" in parentheses. The Bibliography makes no attempt at being complete; we have listed mainly the papers which are discussed in the text.

Finally, we want to thank all those who have helped and encouraged us to prepare this book. The marvellous "Minisymposium" which G. Dahlquist organized in Stockholm in 1979 gave us the first impulse for writing this book. J. Steinig and Chr. Lubich have read the whole manuscript very carefully and have made extremely valuable mathematical and linguistic suggestions. We also thank J.P. Eckmann for his troff software with the help of which the whole manuscript has been printed. For preliminary versions we had used textprocessing programs written by R. Menk. Thanks also to the staff of the Geneva computing center for their help. All computer plots have been done on their beautiful HP plotter. Last but not least, we would like to acknowledge the agreeable collaboration with the planning and production group of Springer-Verlag.

October 29, 1986

The Authors

Preface to the Second Edition

The preparation of the second edition has presented a welcome opportunity to improve the first edition by rewriting many sections and by eliminating errors and misprints. In particular we have included new material on

- Hamiltonian systems (I.14) and symplectic Runge-Kutta methods (II.16);
- dense output for Runge-Kutta (II.6) and extrapolation methods (II.9);
- a new Dormand & Prince method of order 8 with dense output (II.5);
- parallel Runge-Kutta methods (II.11);
- numerical tests for first- and second order systems (II.10 and III.7).

Our sincere thanks go to many persons who have helped us with our work:

- all readers who kindly drew our attention to several errors and misprints in the first edition;
- those who read preliminary versions of the new parts of this edition for their invaluable suggestions: D.J. Higham, L. Jay, P. Kaps, Chr. Lubich, B. Moesli, A. Ostermann, D. Pfenniger, P.J. Prince, and J.M. Sanz-Serna.
- our colleague J. Steinig, who read the entire manuscript, for his numerous mathematical suggestions and corrections of English (and Latin!) grammar;
- our colleague J.P. Eckmann for his great skill in manipulating Apollo workstations, font tables, and the like;
- the staff of the Geneva computing center and of the mathematics library for their constant help;
- the planning and production group of Springer-Verlag for numerous suggestions on presentation and style.

This second edition now also benefits, as did Volume II, from the marvels of \TeX technology. All figures have been recomputed and printed, together with the text, in Postscript. Nearly all computations and text processings were done on the Apollo DN4000 workstation of the Mathematics Department of the University of Geneva; for some long-time and high-precision runs we used a VAX 8700 computer and a Sun IPX workstation.

November 29, 1992

The Authors

Contents

Chapter I. Classical Mathematical Theory

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

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

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

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

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