

Numerical Methods for Ordinary Differential Equations

Numerical Methods for Ordinary Differential Equations

J. C. Butcher

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Contents

Foreword	xiii
Preface to the first edition	xv
Preface to the second edition	xix
Preface to the third edition	xxi
1 Differential and Difference Equations	1
10 Differential Equation Problems	1
100 Introduction to differential equations	1
101 The Kepler problem	4
102 A problem arising from the method of lines	7
103 The simple pendulum	11
104 A chemical kinetics problem	14
105 The Van der Pol equation and limit cycles	16
106 The Lotka–Volterra problem and periodic orbits	18
107 The Euler equations of rigid body rotation	20
11 Differential Equation Theory	22
110 Existence and uniqueness of solutions	22
111 Linear systems of differential equations	24
112 Stiff differential equations	26
12 Further Evolutionary Problems	28
120 Many-body gravitational problems	28
121 Delay problems and discontinuous solutions	30
122 Problems evolving on a sphere	33
123 Further Hamiltonian problems	35
124 Further differential-algebraic problems	36
13 Difference Equation Problems	38
130 Introduction to difference equations	38
131 A linear problem	39
132 The Fibonacci difference equation	40
133 Three quadratic problems	40
134 Iterative solutions of a polynomial equation	41
135 The arithmetic-geometric mean	43

14	Difference Equation Theory	44
140	<i>Linear difference equations</i>	44
141	<i>Constant coefficients</i>	45
142	<i>Powers of matrices</i>	46
15	Location of Polynomial Zeros	50
150	<i>Introduction</i>	50
151	<i>Left half-plane results</i>	50
152	<i>Unit disc results</i>	52
	Concluding remarks	53
2	Numerical Differential Equation Methods	55
20	The Euler Method	55
200	<i>Introduction to the Euler method</i>	55
201	<i>Some numerical experiments</i>	58
202	<i>Calculations with stepsize control</i>	61
203	<i>Calculations with mildly stiff problems</i>	65
204	<i>Calculations with the implicit Euler method</i>	68
21	Analysis of the Euler Method	70
210	<i>Formulation of the Euler method</i>	70
211	<i>Local truncation error</i>	71
212	<i>Global truncation error</i>	72
213	<i>Convergence of the Euler method</i>	73
214	<i>Order of convergence</i>	74
215	<i>Asymptotic error formula</i>	78
216	<i>Stability characteristics</i>	79
217	<i>Local truncation error estimation</i>	84
218	<i>Rounding error</i>	85
22	Generalizations of the Euler Method	90
220	<i>Introduction</i>	90
221	<i>More computations in a step</i>	90
222	<i>Greater dependence on previous values</i>	92
223	<i>Use of higher derivatives</i>	92
224	<i>Multistep–multistage–multiderivative methods</i>	94
225	<i>Implicit methods</i>	95
226	<i>Local error estimates</i>	96
23	Runge–Kutta Methods	97
230	<i>Historical introduction</i>	97
231	<i>Second order methods</i>	98
232	<i>The coefficient tableau</i>	98
233	<i>Third order methods</i>	99
234	<i>Introduction to order conditions</i>	100
235	<i>Fourth order methods</i>	101
236	<i>Higher orders</i>	103
237	<i>Implicit Runge–Kutta methods</i>	103
238	<i>Stability characteristics</i>	104
239	<i>Numerical examples</i>	108

24 Linear Multistep Methods	111
240 <i>Historical introduction</i>	111
241 <i>Adams methods</i>	111
242 <i>General form of linear multistep methods</i>	113
243 <i>Consistency, stability and convergence</i>	113
244 <i>Predictor–corrector Adams methods</i>	115
245 <i>The Milne device</i>	117
246 <i>Starting methods</i>	118
247 <i>Numerical examples</i>	119
25 Taylor Series Methods	120
250 <i>Introduction to Taylor series methods</i>	120
251 <i>Manipulation of power series</i>	121
252 <i>An example of a Taylor series solution</i>	122
253 <i>Other methods using higher derivatives</i>	123
254 <i>The use of f' derivatives</i>	126
255 <i>Further numerical examples</i>	126
26 Multistage Methods	128
260 <i>Historical introduction</i>	128
261 <i>Pseudo Runge–Kutta methods</i>	128
262 <i>Two-step Runge–Kutta methods</i>	129
263 <i>Generalized linear multistep methods</i>	130
264 <i>General linear methods</i>	131
265 <i>Numerical examples</i>	133
27 Introduction to Implementation	135
270 <i>Choice of method</i>	135
271 <i>Variable stepsize</i>	136
272 <i>Interpolation</i>	138
273 <i>Experiments with the Kepler problem</i>	138
274 <i>Experiments with a discontinuous problem</i>	139
Concluding remarks	142
 3 Runge–Kutta Methods	 143
30 Preliminaries	143
300 <i>Trees and rooted trees</i>	143
301 <i>Trees, forests and notations for trees</i>	146
302 <i>Centrality and centres</i>	147
303 <i>Enumeration of trees and unrooted trees</i>	150
304 <i>Functions on trees</i>	153
305 <i>Some combinatorial questions</i>	155
306 <i>Labelled trees and directed graphs</i>	156
307 <i>Differentiation</i>	159
308 <i>Taylor's theorem</i>	161

31 Order Conditions	163
310 <i>Elementary differentials</i>	163
311 <i>The Taylor expansion of the exact solution</i>	166
312 <i>Elementary weights</i>	168
313 <i>The Taylor expansion of the approximate solution</i>	171
314 <i>Independence of the elementary differentials</i>	174
315 <i>Conditions for order</i>	174
316 <i>Order conditions for scalar problems</i>	175
317 <i>Independence of elementary weights</i>	178
318 <i>Local truncation error</i>	180
319 <i>Global truncation error</i>	181
32 Low Order Explicit Methods	185
320 <i>Methods of orders less than 4</i>	185
321 <i>Simplifying assumptions</i>	186
322 <i>Methods of order 4</i>	189
323 <i>New methods from old</i>	195
324 <i>Order barriers</i>	200
325 <i>Methods of order 5</i>	204
326 <i>Methods of order 6</i>	206
327 <i>Methods of order greater than 6</i>	209
33 Runge–Kutta Methods with Error Estimates	211
330 <i>Introduction</i>	211
331 <i>Richardson error estimates</i>	211
332 <i>Methods with built-in estimates</i>	214
333 <i>A class of error-estimating methods</i>	215
334 <i>The methods of Fehlberg</i>	221
335 <i>The methods of Verner</i>	223
336 <i>The methods of Dormand and Prince</i>	223
34 Implicit Runge–Kutta Methods	226
340 <i>Introduction</i>	226
341 <i>Solvability of implicit equations</i>	227
342 <i>Methods based on Gaussian quadrature</i>	228
343 <i>Reflected methods</i>	233
344 <i>Methods based on Radau and Lobatto quadrature</i>	236
35 Stability of Implicit Runge–Kutta Methods	243
350 <i>A-stability, $A(\alpha)$-stability and L-stability</i>	243
351 <i>Criteria for A-stability</i>	244
352 <i>Padé approximations to the exponential function</i>	245
353 <i>A-stability of Gauss and related methods</i>	252
354 <i>Order stars</i>	253
355 <i>Order arrows and the Ehle barrier</i>	256
356 <i>AN-stability</i>	259
357 <i>Non-linear stability</i>	262
358 <i>BN-stability of collocation methods</i>	265
359 <i>The V and W transformations</i>	267

36 Implementable Implicit Runge–Kutta Methods	272
360 <i>Implementation of implicit Runge–Kutta methods</i>	272
361 <i>Diagonally implicit Runge–Kutta methods</i>	273
362 <i>The importance of high stage order</i>	274
363 <i>Singly implicit methods</i>	278
364 <i>Generalizations of singly implicit methods</i>	283
365 <i>Effective order and DESIRE methods</i>	285
37 Implementation Issues	288
370 <i>Introduction</i>	288
371 <i>Optimal sequences</i>	288
372 <i>Acceptance and rejection of steps</i>	290
373 <i>Error per step versus error per unit step</i>	291
374 <i>Control-theoretic considerations</i>	292
375 <i>Solving the implicit equations</i>	293
38 Algebraic Properties of Runge–Kutta Methods	296
380 <i>Motivation</i>	296
381 <i>Equivalence classes of Runge–Kutta methods</i>	297
382 <i>The group of Runge–Kutta tableaux</i>	299
383 <i>The Runge–Kutta group</i>	302
384 <i>A homomorphism between two groups</i>	308
385 <i>A generalization of G_1</i>	309
386 <i>Some special elements of G</i>	311
387 <i>Some subgroups and quotient groups</i>	314
388 <i>An algebraic interpretation of effective order</i>	316
39 Symplectic Runge–Kutta Methods	323
390 <i>Maintaining quadratic invariants</i>	323
391 <i>Hamiltonian mechanics and symplectic maps</i>	324
392 <i>Applications to variational problems</i>	325
393 <i>Examples of symplectic methods</i>	326
394 <i>Order conditions</i>	327
395 <i>Experiments with symplectic methods</i>	328
Concluding remarks	331
 4 Linear Multistep Methods	 333
40 Preliminaries	333
400 <i>Fundamentals</i>	333
401 <i>Starting methods</i>	334
402 <i>Convergence</i>	335
403 <i>Stability</i>	336
404 <i>Consistency</i>	336
405 <i>Necessity of conditions for convergence</i>	338
406 <i>Sufficiency of conditions for convergence</i>	339
41 The Order of Linear Multistep Methods	344
410 <i>Criteria for order</i>	344
411 <i>Derivation of methods</i>	346
412 <i>Backward difference methods</i>	347

42	Errors and Error Growth	348
420	<i>Introduction</i>	348
421	<i>Further remarks on error growth</i>	350
422	<i>The underlying one-step method</i>	352
423	<i>Weakly stable methods</i>	354
424	<i>Variable stepsize</i>	355
43	Stability Characteristics	357
430	<i>Introduction</i>	357
431	<i>Stability regions</i>	359
432	<i>Examples of the boundary locus method</i>	360
433	<i>An example of the Schur criterion</i>	363
434	<i>Stability of predictor–corrector methods</i>	364
44	Order and Stability Barriers	367
440	<i>Survey of barrier results</i>	367
441	<i>Maximum order for a convergent k-step method</i>	368
442	<i>Order stars for linear multistep methods</i>	371
443	<i>Order arrows for linear multistep methods</i>	373
45	One-leg Methods and G-stability	375
450	<i>The one-leg counterpart to a linear multistep method</i>	375
451	<i>The concept of G-stability</i>	376
452	<i>Transformations relating one-leg and linear multistep methods</i>	379
453	<i>Effective order interpretation</i>	380
454	<i>Concluding remarks on G-stability</i>	380
46	Implementation Issues	381
460	<i>Survey of implementation considerations</i>	381
461	<i>Representation of data</i>	382
462	<i>Variable stepsize for Nordsieck methods</i>	385
463	<i>Local error estimation</i>	386
	Concluding remarks	387
5	General Linear Methods	389
50	Representing Methods in General Linear Form	389
500	<i>Multivalued–multistage methods</i>	389
501	<i>Transformations of methods</i>	391
502	<i>Runge–Kutta methods as general linear methods</i>	392
503	<i>Linear multistep methods as general linear methods</i>	393
504	<i>Some known unconventional methods</i>	396
505	<i>Some recently discovered general linear methods</i>	398
51	Consistency, Stability and Convergence	400
510	<i>Definitions of consistency and stability</i>	400
511	<i>Covariance of methods</i>	401
512	<i>Definition of convergence</i>	403
513	<i>The necessity of stability</i>	404
514	<i>The necessity of consistency</i>	404
515	<i>Stability and consistency imply convergence</i>	406

52 The Stability of General Linear Methods	412
520 <i>Introduction</i>	412
521 <i>Methods with maximal stability order</i>	413
522 <i>Outline proof of the Butcher–Chipman conjecture</i>	417
523 <i>Non-linear stability</i>	419
524 <i>Reducible linear multistep methods and G-stability</i>	422
53 The Order of General Linear Methods	423
530 <i>Possible definitions of order</i>	423
531 <i>Local and global truncation errors</i>	425
532 <i>Algebraic analysis of order</i>	426
533 <i>An example of the algebraic approach to order</i>	428
534 <i>The underlying one-step method</i>	429
54 Methods with Runge–Kutta stability	431
540 <i>Design criteria for general linear methods</i>	431
541 <i>The types of DIMSIM methods</i>	432
542 <i>Runge–Kutta stability</i>	435
543 <i>Almost Runge–Kutta methods</i>	438
544 <i>Third order, three-stage ARK methods</i>	441
545 <i>Fourth order, four-stage ARK methods</i>	443
546 <i>A fifth order, five-stage method</i>	446
547 <i>ARK methods for stiff problems</i>	446
55 Methods with Inherent Runge–Kutta Stability	448
550 <i>Doubly companion matrices</i>	448
551 <i>Inherent Runge–Kutta stability</i>	450
552 <i>Conditions for zero spectral radius</i>	452
553 <i>Derivation of methods with IRK stability</i>	454
554 <i>Methods with property F</i>	457
555 <i>Some non-stiff methods</i>	458
556 <i>Some stiff methods</i>	459
557 <i>Scale and modify for stability</i>	460
558 <i>Scale and modify for error estimation</i>	462
56 G-symplectic methods	464
560 <i>Introduction</i>	464
561 <i>The control of parasitism</i>	467
562 <i>Order conditions</i>	471
563 <i>Two fourth order methods</i>	474
564 <i>Starters and finishers for sample methods</i>	476
565 <i>Simulations</i>	480
566 <i>Cohesiveness</i>	481
567 <i>The role of symmetry</i>	487
568 <i>Efficient starting</i>	492
Concluding remarks	497
References	499
Index	509

Foreword

This book is devoted to a subject – the numerical solution of ordinary differential equations – where practical relevance meets mathematical beauty in a unique way. Its writing is masterly, as befits its author, someone whose past and current contributions to the field are second to none in history.

The numerical integration of differential equations plays a crucial role in all applications of mathematics. Virtually all the scientific laws that govern the physical world can be expressed as differential equations; therefore making explicit the implications and consequences of these laws requires finding the solutions to the equations. This necessity, coupled with the unfortunate fact that there is no general rule to solve analytically a given differential equation, has led over the years to the introduction by the best mathematical minds of a raft of techniques applicable only in particular equations or oriented to specific features of the solutions sought. While some of those efforts have significantly spurred the development of mathematics in the last 300 years (e.g. they have given us the theory of special functions, Lie groups and topology), numerical methods are the only master key for solving differential equations.

The subject matter of this volume is not only of exceptional relevance due to its importance in practical applications; it also constitutes a rich and elegant branch of mathematics with exceptionally distinguished roots. As is well known, the simplest numerical algorithm to solve (ordinary) differential equations was suggested by Euler in the mid 18th century. It is less well known that, for Euler, what we now call Euler's method was just a stepping stone in his insightful presentation of the Taylor series method of arbitrary order. Euler also carefully discussed the use of variable order and variable step lengths and implementation details. The next milestone of the subject, the introduction of multistep algorithms, was reached in the mid 19th century by Adams, the scientist best known for having co-discovered the existence of the planet Neptune using only mathematics. Another important class of numerical integrators was introduced by Runge and systematized by Kutta around the year 1900. Thus, 100 years ago, the sciences had a pressing need to solve differential equations, so the mathematicians put forward many useful algorithms to solve them . . . and yet there was a big gap: carrying out the required computations was typically unfeasible when pencil and paper or mechanical machines were the only ways of performing arithmetic operations. It is no exaggeration to state that the need to implement in practice the integration algorithms of Adams, Runge and Kutta led to the conception and construction of (digital, electronic) computers; after all, one the

first computers was named ENIAC, (electronic numerical integrator and computer). Since then, computers have of course revolutionized not only the mathematical solution of differential equations but almost everything else.

It was only natural that when the use of computers became widespread, mathematicians asked themselves whether the venerable integrators introduced by Adams, Runge and Kutta were the best conceivable. As it turned out, in the multistep field, the beautiful mathematics of Dahlquist showed that for nonstiff problems it is not really feasible to do much better than Adams had suggested. By the addition of extra free parameters, it is possible to concoct more sophisticated integrators, but these are doomed to be unstable. In the Runge-Kutta realm the situation is just the opposite: the many degrees of freedom in the world of Runge-Kutta integrators have shown themselves capable of providing a good integrator for each situation.

The construction and analysis of specific Runge-Kutta schemes is a daunting job if one approaches it as Runge and Kutta did; these schemes are highly nonlinear with a remarkable Matrioshka doll structure, where the vector field has to be evaluated at an expression that involves the vector field evaluated at an expression that involves the vector field . . . Mathematics owes much to the author of this book for a simple and elegant, alternative, general methodology based on the use of trees and other algebraic ideas. It is thanks to J. C. Butcher's techniques that many authors have been able in the last decades to develop Runge-Kutta methods tailored to different needs and to implement them in useful software. Many such techniques have found uses away from numerical mathematics in fields such as quantum field theory and noncommutative geometry. Connes (Field medallist 1982) and Kreimer, writing on renormalization theories, state: 'We regard Butcher's work on the classification of numerical integration methods as an impressive example that concrete problem-oriented work can lead to far-reaching conceptual results.'

The author wrote an earlier text restricted to Runge-Kutta and general linear methods. In the case of the present more comprehensive volume, this is the third, significantly updated, edition; I am sure it will be as well received as the two preceding editions.

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Preface to the first edition

Introductory remarks

This book represents an attempt to modernize and expand my previous volume, *The Numerical Analysis of Ordinary Differential Equations: Runge–Kutta and General Linear Methods*. It is more modern in that it considers several topics that had not yet emerged as important research areas when the former book was written. It is expanded in that it contains a comprehensive treatment of linear multistep methods. This achieves a better balance than the earlier volume which made a special feature of Runge–Kutta methods.

In order to accommodate the additional topics, some sacrifices have been made. The background work which introduced the earlier book is here reduced to an introductory chapter dealing only with differential and difference equations. Several topics that seem to be still necessary as background reading are now introduced in survey form where they are actually needed. Some of the theoretical ideas are now explained in a less formal manner. It is hoped that mathematical rigour has not been seriously jeopardized by the use of this more relaxed style; if so, then there should be a corresponding gain in accessibility. It is believed that no theoretical detail has been glossed over to the extent that an interested reader would have any serious difficulty in filling in the gaps.

It is hoped that lowering the level of difficulty in the exposition will widen the range of readers who might be able to find this book interesting and useful. With the same idea in mind, exercises have been introduced at the end of each section.

Following the chapter on differential and difference equations, Chapter 2 is presented as a study of the Euler method. However, it aims for much more than this in that it also reviews many other methods and classes of methods as generalizations of the Euler method. This chapter can be used as a broad-ranging introduction to the entire subject of numerical methods for ordinary differential equations.

Chapter 3 contains a detailed analysis of Runge–Kutta methods. It includes studies of the order, stability and convergence of Runge–Kutta methods and also considers in detail the design of efficient explicit methods for non-stiff problems. For implicit methods for stiff problems, inexpensive implementation costs must be added to accuracy and stability as a basic requirement. Recent work on each of these questions is surveyed and discussed.

Linear multistep methods, including the combination of two methods as predictor–corrector pairs, are considered in Chapter 4. The theory interrelating stability, consistency and convergence is presented together with an analysis of order conditions. This leads to a proof of the (first) ‘Dahlquist barrier’. The methods in this class which are generally considered to be the most important for the practical solution of non-stiff problems are the Adams–Bashforth and Adams–Moulton formulae. These are discussed in detail, including their combined use as predictor–corrector pairs. The application of linear multistep methods to stiff problems is also of great practical importance and the treatment will include an analysis of the backward difference formulae.

In Chapter 5 the wider class of general linear methods is introduced and analysed. Questions analogous to those arising in the classical Runge–Kutta and linear multistep methods – that is, questions of consistency, stability, convergence and order – are considered and explored. Several sub-families of methods, that have a potential practical usefulness, are examined in detail. This includes the so-called DIMSIM methods and a new type of method exhibiting what is known as inherent Runge–Kutta stability.

The remarks in the following paragraphs are intended to be read following Chapter 5.

Concluding remarks

Any account of this rapidly evolving subject is bound to be incomplete. Complete books are all alike; every incomplete book is incomplete in its own way.

It has not been possible to deal adequately with implementation questions. Numerical software for evolutionary problems entered its modern phase with the DIFSUB code of Gear (1971b). ‘Modern’ in this sense means that most of the ingredients of subsequent codes were present. Both stiff and non-stiff problems are catered for, provision is made for Jacobian calculation either by subroutine call or by difference approximation; the choice is up to the user. Most important, automatic selection of stepsize and order is made dynamically as the solution develops. Compared with this early implementation of linear multistep methods, the Radau code (Hairer and Wanner 1996) uses implicit Runge–Kutta methods for the solution of stiff problems.

In recent years, the emphasis in numerical methods for evolutionary problems has moved beyond the traditional areas of non-stiff and stiff problems. In particular, differential algebraic equations have become the subject of intense analysis as well as the development of reliable and efficient algorithms for problems of variable difficulty, as measured for example by the indices of the problems. Some basic references in this vibrant area are Brenan, Campbell and Petzold (1996) and Hairer, Lubich and Roche (1989). In particular, many codes are now designed for applications to stiff ordinary differential equations in which algebraic constraints also play a role. On the Runge–Kutta side, Radau is an example of this multipurpose approach. On the linear multistep side, Petzold’s DASSL code is closely related

to Gear's DIFSUB code but has the capability of solving differential algebraic equations, at least of low index.

Many problems derived from mechanical systems can be cast in a Hamiltonian formulation. To faithfully model the behaviour of such problems it is necessary to respect the symplectic structure. Early work on this by the late Feng Kang has led to worldwide activity in the study of this type of question. A basic reference on Hamiltonian problems is Sanz-Serna and Calvo (1994)

The emphasis on the preservation of qualitative features of a numerical solution has now grown well beyond the Hamiltonian situation and has become a mathematical discipline in its own right. We mention just two key references in this emerging subject of 'geometric integration'. They are Iserles et al. (2000) and Hairer, Lubich and Wanner (2006).

Internet commentary

Undoubtedly there will be comments and suggestions raised by readers of this volume. A web resource has been developed to form a commentary and information exchange for issues as they arise in the future. The entry point is

<http://www.math.auckland.ac.nz/~butcher/book>

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During part of the time I have been working on this book, I have received a grant from the Marsden Fund. I am very grateful for this assistance both as an expression of confidence from my scientific colleagues in New Zealand and as practical support.

The weekly workshop in numerical analysis at The University of Auckland has been an important activity in the lives of many students, colleagues and myself. We sometimes refer to this workshop as the 'Runge–Kutta Club'. Over the past five or more years especially, my participation in this workshop has greatly added to my understanding of numerical analysis through collaboration and vigorous discussions. As this book started to take shape they have provided a sounding board for many ideas, some of which were worked on and improved and some of which were ultimately discarded. Many individual colleagues, both in Auckland and overseas, have read and worked through drafts of the book at various stages of its development. Their comments have been invaluable to me and I express my heartfelt thanks.

Amongst my many supportive colleagues, I particularly want to name Christian Brouder, Robert Chan, Tina Chan, David Chen, Allison Heard, Shirley Huang, Arie Iserles, Zdzisław Jackiewicz, Pierre Leone, Taketomo (Tom) Mitsui, Nicolette Moir, Steffen Schulz, Anjana Singh, Angela Tsai, Priscilla Tse and Will Wright.

Preface to the second edition

Reintroductory remarks

The incremental changes incorporated into this edition are an acknowledgement of progress in several directions. The emphasis on structure-preserving algorithms has driven much of this recent progress, but not all of it. The classical linear multistep and Runge–Kutta methods have always been special cases of the large family of general linear methods, but this observation is of no consequence unless some good comes of it. In my opinion, there are only two good things that might be worth achieving. The first is that exceptionally good methods might come to light which would not have been found in any other way. The second is that a clearer insight and perhaps new overarching theoretical results might be expressed in the general linear setting. I believe that both these aims have been achieved, but other people might not agree. However, I hope it can be accepted that some of the new methods which arise naturally as general linear methods have at least some potential in practical computation. I hope also that looking at properties of traditional methods from within the general linear framework will provide additional insight into their computational properties.

How to read this book

Of the five chapters of this book, the first two are the most introductory in nature. Chapter 1 is a review of differential and difference equations with a systematic study of their basic properties balanced against an emphasis on interesting and prototypical problems. Chapter 2 provides a broad introduction to numerical methods for ordinary differential equations. This is motivated by the simplicity of the Euler method and a view that other standard methods are systematic generalizations of this basic method. If Runge–Kutta and linear multistep methods are generalizations of Euler then so are general linear methods, and it is natural to introduce a wide range of multivalued-multistage methods at this elementary level.

A reading of this book should start with these two introductory chapters. For a reader less experienced in this subject this is an obvious entry point but they also have a role for a reader who is ready to go straight into the later chapters. For such readers, they will not take very long but they do set the scene for an entry into the most technical parts of the book.

Chapter 3 is intended as a comprehensive study of Runge–Kutta methods. A full theory of order and stability is presented and at least the early parts of this chapter are prerequisites for Chapter 5 and to a lesser extent for Chapter 4. The use of B-series, or the coefficients that appear in these series, is becoming more and more a standard tool for a full understanding of modern developments in this subject.

Chapter 4 is a full study of linear multistep methods. It is based on Dahlquist’s classic work on consistency, stability and order and includes analysis of linear and nonlinear stability. In both Chapters 3 and 4 the use of order stars to resolve order and stability questions is complemented by the introduction of order arrows. It is probably a good idea to read through most of Chapter 4 before embarking on Chapter 5. This is not because general linear methods are intrinsically inaccessible, but because an appreciation of their overarching nature hinges on an appreciation of the special cases they include.

General linear methods, the subject of Chapter 5, treat well-known methods in a unified way, but it is hoped that they do more than this. There really seem to be new and useful methods buried amongst them which cannot be easily motivated in any other way. Thus, while this chapter needs to be put aside to be read as a culmination, it should not be put off too long. There is so much nice mathematics already associated with these methods, and the promise of more to come provides attraction enough. It is general linear methods, and the stability functions associated with them, that really put order arrows in their rightful place.

Internet support pages

For additional information and supporting material see

<http://www.math.auckland.ac.nz/~butcher/ODE-book-2008>

Reacknowledgements

I have many people to thank and to rethank in my efforts to produce an improved edition. My understanding of the stability and related properties of general linear methods has been sharpened by working with Adrian Hill and Laura Hewitt. Helmut Podhaisky has given me considerable help and advice, especially on aspects of general linear method implementation. My special thanks to Jane Lee for assistance with the final form of the manuscript. A number of people have made comments and provided corrections on the first edition or made constructive suggestions on early drafts of this new version. In addition to people acknowledged in some other way, I would like to mention the names of Ian Gladwell, Dawoomi Kim, Yoshio Komori, René Lamour, Dione O’Neale, Christian Perret, Higinio Ramos, Dave Simpson, Steve Stalos, Caren Tischendorf, Daniel Weiß, Frank Wrona and Jinsen Zhuang.

Preface to the third edition

A new edition

‘Numerical methods for ordinary differential equations’ is a mature and stable subject, and new ideas and techniques should not be expected too frequently. While this new edition is a consolidation of the early editions, it does attempt to take the subject further in some directions. Most notably, Section 56, dealing with G-symplectic methods, records some major advances in what is now known about these methods. At the time of the appearance of the second edition the author, and people with whom he was collaborating, did not fully appreciate the disastrous role that parasitism could play in extended time integrations. This shortcoming has now been overcome. In Butcher, Habib, Hill and Norton (2014), parasitism has been analysed and largely dealt with as a source of numerical difficulty. A recent result (Butcher 2015) has gone some way towards explaining why G-symplectic methods work as well as they do. However, D’Ambrosio and Hairer (2014) show that the suppression of unstable behaviour caused by parasitism cannot be relied on forever. This third edition attempts to present this new work in a manner that underlines the potential of G-symplectic methods as practical integrators for Hamiltonian and other problems. Although known G-symplectic methods are generally restricted to order 4, a new result (Butcher, Imran and Podhaisky 2016) shows how order 6 methods can be constructed. Limited numerical testing confirms the order and conservation properties of this new method and one of these tests is quoted as Figure 568(ii).

Chapter 3 played a central role in the previous editions and does so again. The aspects of this subject, dealing with the composition group, will be difficult for some readers and this edition attempts to explain this in a fresh way. But the importance of algebraic analysis, or anything else of a theoretical nature, must, to a large extent, be in the applications. This theory is not merely a mathematical device; it leads to the construction of useful numerical methods and gives insight to the nature of these methods.

Attributions and personal names

Many results in numerical analysis began as conjectures and were eventually proved, but not always by the individuals who formulated the conjectures. For example, the Ehle (Ehle 1973) and Daniel Moore (Daniel and Moore 1970) conjectures were not

settled until the invention of order stars (Wanner, Hairer and Nørsett 1978). In this volume I have tried to use the convention of naming these results using the names of the first people to formulate them because I believe this avoids confusion about which result is being referred to.

Some authors refer to the commonly used tableaux of coefficients in a specific Runge–Kutta methods as ‘Butcher tableaux’. In this third edition I sometimes follow this terminology but the single word ‘tableau’ is usually enough to make it clear what is being referred to in any particular case. There are many different products associated with rooted trees, the most important being used for the constructing of forests as the product of trees. However, in this book, extensive use is made of the product $t_1 \circ t_2$ formed by adjoining the two roots and defining the root of the product as the same vertex as the root of t_1 . This is sometimes referred to as the ‘Butcher product’ and this name will be used in this edition.

The late Germund Dahlquist once told me why he used the name ‘A-stability’ for this fundamental linear stability definition. It was simply to follow the lead of David M. Young who used ‘property A’ as the name of a fundamental condition in an entirely different area of numerical analysis. When Germund introduced the nonlinear definition ‘G-stability’, he was referring to the matrix G which appears in the formulation of the concept. Shortly afterwards I needed a name for nonlinear stability in the case of Runge–Kutta methods, and I chose B because it next follows A. The fact that B is one of my initials is no more significant than the fact that G is one of the initials of Germund Dahlquist.

Algorithms

The purpose of including formal algorithms in this book is to illuminate the numerical processes they represent. Hence, they should not be interpreted as computer codes. Nevertheless, with little or no change, they can be used as scripts or functions in a variety of languages including MATLAB®, Octave and Scilab.

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for amplitudes greater than $\pi/2$, parasitism eventually produces disastrous effects. Ernst kindly sent me his own analysis of this phenomenon.

Many colleagues throughout the world have discussed interesting questions with me, and I am grateful for these stimulating interactions. There are too many to name individually but I do want to make a special mention of the colleagues and former students who have collaborated with me and learnt with me about G-symplectic and other types of general linear methods: Saghir Ahmad, Yousaf Habib, Adrian Hill, Gulshad Imran, Terrence Norton and Helmut Podhaisky.

Over the years, including the period when I worked on this new edition, I have received generous support from the Marsden Fund and this has given me opportunities I would not otherwise have had.

I have enjoyed the support of children, stepchildren and grandchildren in all aspects of my life. I express my special appreciation for the nest Jennifer has provided for me: a bower ‘full of sweet dreams, and health, and quiet breathing’.