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E.Hairer G.Wanner

Solving Ordinary Differential Equations II

Stiff and Differential -Algebraic Problems

Second Edition

常微分方程的解法II

刚性与微分代数问题

(第二版)

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《国外数学名著系列》(影印版)序

要使我国的数学事业更好地发展起来,需要数学家淡泊名利并付出更艰苦地努力。另一方面,我们也要从客观上为数学家创造更有利的发展数学事业的外部环境,这主要是加强对数学事业的支持与投资力度,使数学家有较好的工作与生活条件,其中也包括改善与加强数学的出版工作。

从出版方面来讲,除了较好较快地出版我们自己的成果外,引进国外的先进出版物无疑也是十分重要与必不可少的。从数学来说,施普林格(Springer)出版社至今仍然是世界上最具权威的出版社。科学出版社影印一批他们出版的好的新书,使我国广大数学家能以较低的价格购买,特别是在边远地区工作的数学家能普遍见到这些书,无疑是对推动我国数学的科研与教学十分有益的事。

这次科学出版社购买了版权,一次影印了23本施普林格出版社出版的数学书,就是一件好事,也是值得继续做下去的事情。大体上分一下,这23本书中,包括基础数学书5本,应用数学书6本与计算数学书12本,其中有些书也具有交叉性质。这些书都是很新的,2000年以后出版的占绝大部分,共计16本,其余的也是1990年以后出版的。这些书可以使读者较快地了解数学某方面的前沿,例如基础数学中的数论、代数与拓扑三本,都是由该领域大数学家编著的“数学百科全书”的分册。对从事这方面研究的数学家了解该领域的前沿与全貌很有帮助。按照学科的特点,基础数学类的书以“经典”为主,应用和计算数学类的书以“前沿”为主。这些书的作者多数是国际知名的大数学家,例如《拓扑学》一书的作者诺维科夫是俄罗斯科学院的院士,曾获“菲尔兹奖”和“沃尔夫数学奖”。这些大数学家的著作无疑将会对我国的科研人员起到非常好的指导作用。

当然,23本书只能涵盖数学的一部分,所以,这项工作还应该继续做下去。更进一步,有些读者面较广的好书还应该翻译成中文出版,使之有更大的读者群。

总之,我对科学出版社影印施普林格出版社的部分数学著作这一举措表示热烈的支持,并盼望这一工作取得更大的成绩。

王 元

2005年12月3日

To Evi and Myriam

From the Preface to the First Edition

"Whatever regrets may be, we have done our best."

(Sir Ernest Shackleton, turning back on 9 January 1909 at $88^{\circ} 23'$ South.)

Brahms struggled for 20 years to write his first symphony. Compared to this, the 10 years we have been working on these two volumes may even appear short.

This second volume treats stiff differential equations and differential algebraic equations. It contains three chapters: Chapter IV on one-step (Runge-Kutta) methods for stiff problems, Chapter V on multistep methods for stiff problems, and Chapter VI on singular perturbation and differential-algebraic equations.

Each chapter is divided into sections. Usually the first sections of a chapter are of an introductory nature, explain numerical phenomena and exhibit numerical results. Investigations of a more theoretical nature are presented in the later sections of each chapter.

As in Volume I, the formulas, theorems, tables and figures are numbered consecutively in each section and indicate, in addition, the section number. In cross references to other chapters the (latin) chapter number is put first. References to the bibliography are again by "author" plus "year" in parentheses. The bibliography again contains only those papers which are discussed in the text and is in no way meant to be complete.

It is a pleasure to thank J. Butcher, G. Dahlquist, and S.P. Nørsett (coauthor of Volume I) for their interest in the subject and for the numerous discussions we had with them which greatly inspired our work. Special thanks go to the participants of our seminar in Geneva, in particular Ch. Lubich, A. Ostermann and M. Roche, where all the subjects of this book have been presented and discussed over the years. Much help in preparing the manuscript was given by J. Steinig, Ch. Lubich and A. Ostermann who read and re-read the whole text and made innumerable corrections and suggestions for improvement. We express our sincere gratitude to them. Many people have seen particular sections and made invaluable suggestions and remarks: M. Crouzeix, P. Deufhard, K. Gustafsson, G. Hall, W. Hundsdorfer, L. Jay, R. Jeltsch, J.P. Kauthen, H. Kraaijevanger, R. März, and O. Nevanlinna. . . . Several pictures were produced by our children Klaudia Wanner and Martin Hairer, the one by drawing the other by hacking.

The marvellous, perfect and never failing TEX program of D. Knuth allowed us to deliver a camera-ready manuscript to Springer Verlag, so that the book could be produced rapidly and at a reasonable price. We acknowledge with pleasure the numerous remarks of the planning and production group of Springer Verlag concerning fonts, style and other questions of elegance.

March, 1991

The Authors

Preface to the Second Edition

The preparation of the second edition allowed us to improve the first edition by rewriting many sections and by eliminating errors and misprints which have been discovered. In particular we have included new material on

- methods with extended stability (Chebyshev methods) (Sect. IV.2);
 - improved computer codes and new numerical tests for one- and multistep methods (Sects. IV.10 and V.5);
 - new results on properties of error growth functions (Sects. IV.11 and IV.12);
 - quasilinear differential equations with state-dependent mass matrix (Sect. VI.6).
- We have completely reorganized the chapter on differential-algebraic equations by including three new sections on
- index reduction methods (Sect. VII.2);
 - half-explicit methods for index-2 systems (Sect. VII.6);
 - symplectic methods for constrained Hamiltonian systems and backward error analysis on manifolds (Sect. VII.8).

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, in particular C. Bendtsen, R. Chan, P. Chartier, T. Eirola, L. Jay, P. Kaps, J.-P. Kauthen, P. Leone, S. Maset, B. Owren, and L.F. Shampine;
- those who read preliminary versions of the new parts of this edition for their invaluable suggestions: M. Arnold, J. Cash, D.J. Higham, P. Kunkel, Chr. Lubich, A. Medovikov, A. Murua, A. Ostermann, and J. Verwer.
- 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.

All figures have been recomputed and printed, together with the text, in Postscript. All computations and text processings were done on the SUN workstations of the Mathematics Department of the University of Geneva.

April 1996

The Authors

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Chapter IV. Stiff Problems – One-Step Methods

This chapter introduces stiff (styv (Swedish first!), steif (German), stíf (Islandic), stijf (Dutch), raide (French), rígido (Spanish), rígrado (Portuguese), stiff (Italian), kankea (Finnish), δύσκαμπτο (Greek), merev (Hungarian), rigid (Rumanian), tog (Slovenian), čvrst (Serbo-Croatian), tuhý (Czecho-Slovakian), sztywny (Polish), jäik (Estonian), stiegrs (Latvian), standus (Lithuanian), stign (Breton), zurrun (Basque), sert (Turkish), жесткий (Russian), ТВЪРД (Bulgarian), קשיח (Hebrew), ساق (Arabic), سخت (Urdu), سخت (Persian), कठिण (Sanskrit), कठ (Hindi), 刚性 (Chinese), 硬い (Japanese), cứng (Vietnamese), ngumu (Swaheli) . . .) differential equations. While the intuitive meaning of stiff is clear to all specialists, much controversy is going on about it's correct mathematical definition (see e.g. p.360-363 of Aiken (1985)). The most pragmatical opinion is also historically the first one (Curtiss & Hirschfelder 1952): *stiff equations are equations where certain implicit methods, in particular BDF, perform better, usually tremendously better, than explicit ones*. The eigenvalues of the Jacobian $\partial f / \partial y$ play certainly a role in this decision, but quantities such as the dimension of the system, the smoothness of the solution or the integration interval are also important (Sections IV.1 and IV.2).

Stiff equations need new concepts of stability (A-stability, Sect. IV.3) and lead to mathematical theories on order restrictions (order stars, Sect. IV.4). Stiff equations require implicit methods; we therefore focus in Sections IV.5 and IV.6 on implicit Runge-Kutta methods, in IV.7 on (semi-implicit) Rosenbrock methods and in IV.9 on semi-implicit extrapolation methods. The actual efficient implementation of implicit Runge-Kutta methods poses a number of problems which are discussed in Sect. IV.8. Section IV.10 then reports on some numerical experience for all these methods.

With Sections IV.11, IV.12 and IV.13 we begin with the discussion of contractivity (*B*-stability) for linear and nonlinear differential equations. The chapter ends with questions of existence and numerical stability of the implicit Runge-Kutta solutions (Sect. IV.14) and a convergence theory which is independent of the stiffness (*B*-convergence, Sect. IV.15).

IV.1 Examples of Stiff Equations

... Around 1960, things became completely different and everyone became aware that the world was full of stiff problems.

(G. Dahlquist in Aiken 1985)

Stiff equations are problems for which explicit methods don't work. Curtiss & Hirschfelder (1952) explain stiffness on one-dimensional examples such as

$$y' = -50(y - \cos x). \quad (1.1)$$

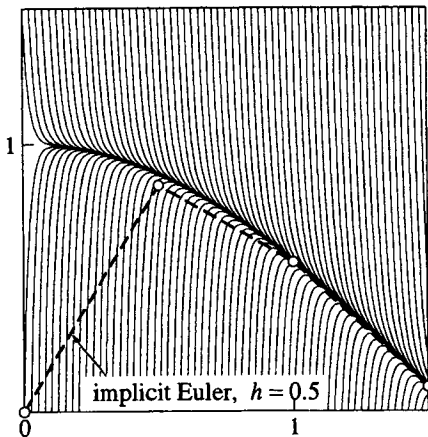


Fig. 1.1. Solution curves of (1.1) with implicit Euler solution

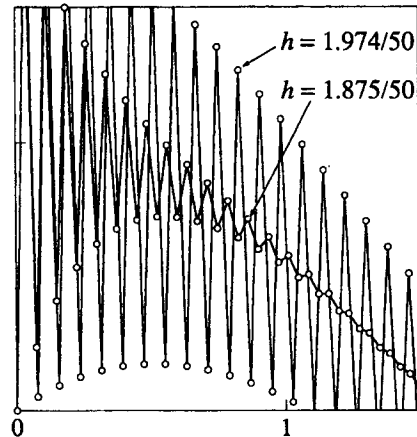


Fig. 1.2. Explicit Euler for $y(0) = 0$, $h = 1.974/50$ and $1.875/50$

Solution curves of Equation (1.1) are shown in Fig. 1.1. There is apparently a smooth solution in the vicinity of $y \approx \cos x$ and all other solutions reach this one after a rapid “transient phase”. Such transients are typical of stiff equations, but are neither sufficient nor necessary. For example, the solution with initial value $y(0) = 1$ (more precisely $2500/2501$) has *no* transient. Fig. 1.2 shows Euler polygons for the initial value $y(0) = 0$ and step sizes $h = 1.974/50$ (38 steps) and $h = 1.875/50$ (40 steps). We observe that whenever the step size is a little too large (larger than $2/50$), the numerical solution goes too far beyond the equilibrium and violent oscillations occur.

Looking for better methods for differential equations such as (1.1), Curtiss and Hirschfelder discovered the BDF method (see Sect. III.1): the approximation

$y \approx \cos x$ (i.e., $f(x, y) = 0$) is only a crude approximation to the smooth solution, since the derivative of $\cos x$ is not zero. It is much better, for a given solution value y_n , to search for a point y_{n+1} where the slope of the vector field is directed towards y_n , hence

$$\frac{y_{n+1} - y_n}{h} = f(x_{n+1}, y_{n+1}). \quad (1.2)$$

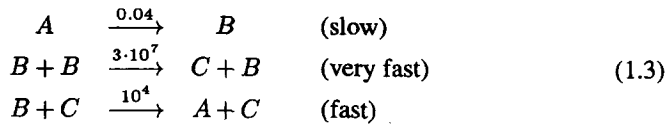
This is the implicit Euler method. The dotted line in Fig. 1.1 consists of three implicit Euler steps and demonstrates impressively the good stability property of this method. Equation (1.1) is thus apparently “stiff” in the sense of Curtiss and Hirschfelder.

Extending the above idea “by taking higher order polynomials to fit y at a large number of points” then leads to the BDF methods.

Chemical Reaction Systems

When the equations represent the behaviour of a system containing a number of fast and slow reactions, a forward integration of these equations becomes difficult. (H.H. Robertson 1966)

The following example of Robertson’s (1966) has become very popular in numerical studies (Willoughby 1974):



which leads to the equations

$$\begin{array}{lll} \text{A:} & y_1' = -0.04y_1 + 10^4 y_2 y_3 & y_1(0) = 1 \\ \text{B:} & y_2' = 0.04y_1 - 10^4 y_2 y_3 - 3 \cdot 10^7 y_2^2 & y_2(0) = 0 \\ \text{C:} & y_3' = 3 \cdot 10^7 y_2^2 & y_3(0) = 0. \end{array} \quad (1.4)$$

After a bad experience with explicit Euler just before, let’s try a higher order method and a more elaborate code for this example: DOPRI5 (cf. Volume 1). The numerical solutions obtained for y_2 with $Rtol = 10^{-2}$ (209 steps) as well as with $Rtol = 10^{-3}$ (205 steps) and $Atol = 10^{-6} \cdot Rtol$ are displayed in Fig. 1.3. Fig. 1.4 presents the step sizes used by the code and also the local error estimates. There, all rejected steps are crossed out.

We observe that the solution y_2 rapidly reaches a quasi-stationary position in the vicinity of $y_2' = 0$, which in the beginning ($y_1 = 1, y_3 = 0$) is at $0.04 \approx 3 \cdot 10^7 y_2^2$, hence $y_2 \approx 3.65 \cdot 10^{-5}$, and then very slowly goes back to zero again. The numerical method, however, integrates this smooth solution by thousands of apparently unnecessary steps. Moreover, the chosen step sizes are more or less independent of the chosen tolerance. Hence, they seem to be governed by stability