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Geometric Numerical Integration

Structure-Preserving Algorithms for Ordinary Differential Equations

Second Edition

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With 146 Figures

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Preface to the First Edition

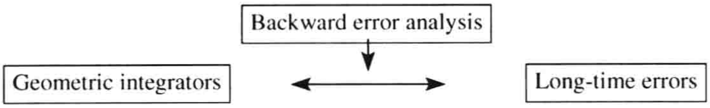
> They throw geometry out the door, and it comes back through the window.
> (H.G.Forder, Auckland 1973, reading new mathematics at the age of 84)

The subject of this book is numerical methods that preserve geometric properties of the flow of a differential equation: symplectic integrators for Hamiltonian systems, symmetric integrators for reversible systems, methods preserving first integrals and numerical methods on manifolds, including Lie group methods and integrators for constrained mechanical systems, and methods for problems with highly oscillatory solutions. Structure preservation – with its questions as to where, how, and what for – is the unifying theme.

In the last few decades, the theory of numerical methods for general (non-stiff and stiff) ordinary differential equations has reached a certain maturity, and excellent general-purpose codes, mainly based on Runge–Kutta methods or linear multistep methods, have become available. The motivation for developing structure-preserving algorithms for special classes of problems came independently from such different areas of research as astronomy, molecular dynamics, mechanics, theoretical physics, and numerical analysis as well as from other areas of both applied and pure mathematics. It turned out that the preservation of geometric properties of the flow not only produces an improved qualitative behaviour, but also allows for a more accurate long-time integration than with general-purpose methods.

An important shift of view-point came about by ceasing to concentrate on the numerical approximation of a single solution trajectory and instead to consider a numerical method as a *discrete dynamical system* which approximates the flow of the differential equation – and so the geometry of phase space comes back again through the window. This view allows a clear understanding of the preservation of invariants and of methods on manifolds, of symmetry and reversibility of methods, and of the symplecticity of methods and various generalizations. These subjects are presented in Chapters IV through VII of this book. Chapters I through III are of an introductory nature and present examples and numerical integrators together with important parts of the classical order theories and their recent extensions. Chapter VIII deals with questions of numerical implementations and numerical merits of the various methods.

It remains to explain the relationship between geometric properties of the numerical method and the favourable error propagation in long-time integrations. This



is done using the idea of *backward error analysis*, where the numerical one-step map is interpreted as (almost) the flow of a modified differential equation, which is constructed as an asymptotic series (Chapter IX). In this way, geometric properties of the numerical integrator translate into structure preservation on the level of the modified equations. Much insight and rigorous error estimates over long time intervals can then be obtained by combining this backward error analysis with KAM theory and related perturbation theories. This is explained in Chapters X through XII for Hamiltonian and reversible systems. The final Chapters XIII and XIV treat the numerical solution of differential equations with high-frequency oscillations and the long-time dynamics of multistep methods, respectively.

This book grew out of the lecture notes of a course given by Ernst Hairer at the University of Geneva during the academic year 1998/99. These lectures were directed at students in the third and fourth year. The reactions of students as well as of many colleagues, who obtained the notes from the Web, encouraged us to elaborate our ideas to produce the present monograph.

We want to thank all those who have helped and encouraged us to prepare this book. In particular, Martin Hairer for his valuable help in installing computers and his expertise in Latex and Postscript, Jeff Cash and Robert Chan for reading the whole text and correcting countless scientific obscurities and linguistic errors, Haruo Yoshida for making many valuable suggestions, Stéphane Cirilli for preparing the files for all the photographs, and Bernard Dudez, the irreplaceable director of the mathematics library in Geneva. We are also grateful to many friends and colleagues for reading parts of the manuscript and for valuable remarks and discussions, in particular to Assyr Abdulle, Melanie Beck, Sergio Blanes, John Butcher, Mari Paz Calvo, Begoña Cano, Philippe Chartier, David Cohen, Peter Deuflhard, Stig Faltinsen, Francesco Fassò, Martin Gander, Marlis Hochbruck, Bulent Karasözen, Wilhelm Kaup, Ben Leimkuhler, Pierre Leone, Frank Loose, Katina Lorenz, Robert McLachlan, Ander Murua, Alexander Ostermann, Truong Linh Pham, Sebastian Reich, Chus Sanz-Serna, Zaijiu Shang, Yifa Tang, Matt West, Will Wright.

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Geneva and Tübingen, November 2001 The Authors

Preface to the Second Edition

The fast development of the subject – and the fast development of the sales of the first edition of this book – has given the authors the opportunity to prepare this second edition. First of all we have corrected several misprints and minor errors which we have discovered or which have been kindly communicated to us by several readers and colleagues. We cordially thank all of them for their help and for their interest in our work. A major point of confusion has been revealed by Robert McLachlan in his book review in SIAM Reviews.

Besides many details, which have improved the presentation throughout the book, there are the following major additions and changes which make the book about 130 pages longer:

- a more prominent place of the Störmer–Verlet method in the exposition and the examples of the first chapter;
- a discussion of the Hénon–Heiles model as an example of a chaotic Hamiltonian system;
- a new Sect. IV.9 on geometric numerical linear algebra considering differential equations on Stiefel and Grassmann manifolds and dynamical low-rank approximations;
- a new improved composition method of order 10 in Sect. V.3;
- a characterization of B-series methods that conserve quadratic first integrals and a criterion for conjugate symplecticity in Sect. VI.8;
- the section on volume preservation taken from Chap. VII to Chap. VI;
- an extended and more coherent Chap. VII, renamed Non-Canonical Hamiltonian Systems, with more emphasis on the relationships between Hamiltonian systems on manifolds and Poisson systems;
- a completely reorganized and augmented Sect. VII.5 on the rigid body dynamics and Lie–Poisson systems;
- a new Sect. VII.6 on reduced Hamiltonian models of quantum dynamics and Poisson integrators for their numerical treatment;
- an improved step-size control for reversible methods in Sects. VIII.3.2 and IX.6;
- extension of Sect. IX.5 on modified equations of methods on manifolds to include constrained Hamiltonian systems and Lie–Poisson integrators;
- reorganization of Sects. IX.9 and IX.10; study of non-symplectic B-series methods that have a modified Hamiltonian, and counter-examples for symmetric methods showing linear growth in the energy error;

- a more precise discussion of integrable reversible systems with new examples in Chap. XI;
- extension of Chap. XIII on highly oscillatory problems to systems with several constant frequencies and to systems with non-constant mass matrix;
- a new Chap. XIV on oscillatory Hamiltonian systems with time- or solution-dependent high frequencies, emphasizing adiabatic transformations, adiabatic invariants, and adiabatic integrators;
- a completely rewritten Chap. XV with more emphasis on linear multistep methods for second order differential equations; a complete backward error analysis including parasitic modified differential equations; a study of the long-time stability and a rigorous explanation of the long-time near-conservation of energy and angular momentum.

Let us hope that this second revised edition will again meet good acceptance by our readers.

Geneva and Tübingen, October 2005 The Authors

Table of Contents

Chapter I.
Examples and Numerical Experiments

This chapter introduces some interesting examples of differential equations and illustrates different types of qualitative behaviour of numerical methods. We deliberately consider only very simple numerical methods of orders 1 and 2 to emphasize the qualitative aspects of the experiments. The same effects (on a different scale) occur with more sophisticated higher-order integration schemes. The experiments presented here should serve as a motivation for the theoretical and practical investigations of later chapters. The reader is encouraged to repeat the experiments or to invent similar ones.

I.1 First Problems and Methods

> Numerical applications of the case of two dependent variables are not easily obtained. (A.J. Lotka 1925, p. 79)

Our first problems, the Lotka–Volterra model and the pendulum equation, are differential equations in two dimensions and show already many interesting geometric properties. Our first methods are various variants of the Euler method, the midpoint rule, and the Störmer–Verlet scheme.

I.1.1 The Lotka–Volterra Model

We start with an equation from mathematical biology which models the growth of animal species. If a real variable $u(t)$ is to represent the number of individuals of a certain species at time t, the simplest assumption about its evolution is $du/dt = u{\cdot}\alpha$, where α is the reproduction rate. A constant α leads to exponential growth. In the case of more species living together, the reproduction rates will also depend on the population numbers of the *other* species. For example, for two species with $u(t)$ denoting the number of predators and $v(t)$ the number of prey, a plausible assumption is made by the *Lotka–Volterra model*

$$\begin{aligned} \dot u &= u(v-2) \\ \dot v &= v(1-u), \end{aligned} \tag{1.1}$$

where the dots on u and v stand for differentiation with respect to time. (We have chosen the constants 2 and 1 in (1.1) arbitrarily.) A.J. Lotka (1925, Chap. VIII) used

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