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A concise introduction to geometric numerical integration. 2nd edition. (English)

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The paradigm of geometric numerical integration is that during the solution of a differential equation, the numerical method should respect certain properties that the exact solution is known to satisfy. This may be a (time) symmetry, a positivity, or keeping a constant volume, mass, energy, etc., or a simple symplectic property. Especially the latter gets particular interest in this book and it means the following. Consider a Hamiltonian system $\dot{x} = f(x)$ with $x = (q, p)$ denoting the vector of the phase variables (position and momentum), then a numerical method ψ_h with steplength h is symplectic if the area of a domain in phase space is constant in every step of the solution method.

The first chapter recalls a number of classical methods (Euler, Heun, trapezium and midpoint rule) to solve differential equations and discusses their properties, while introducing the relevant concepts (order, stability, stiffness,...). These methods are illustrated on simple examples (harmonic oscillator, Hamiltonian systems) and eventually the geometric principle (symplectic versions) of these elementary methods is introduced. This is further extended in the second chapter for higher order methods (like Runge-Kutta) and how they can be adapted to preserve invariants.

Chapter 3 introduces splitting and composition techniques applied to simple methods to give higher order methods. The additive splitting of the right-hand side $f(x)$ will result in a decomposition of the numerical method. The effect of the technique or what order can be achieved depends both on the numerical method used and the application at hand.

The next chapter illustrates several alternatives to generate geometric numerical methods: using generating functions, variational principles, Lie group methods, and linear combination of splitting methods.

Chapter 5 gives an analysis of how these geometric integrators influence the error propagation, especially when integrating over a long time.

In Chapter 6, the splitting and decomposition methods of Chapter 3 are applied to some partial differential equations (Schrödinger and other evolution equations). A space discretization and finite differences or a pseudo spectral method for the time variable leads to (large scale) differential equations that can be solved using geometric integrators.

In a final Chapter 7, some practical examples (N-body problem, Hamiltonian Monte Carlo and Hamiltonian simulation in quantum computing) illustrate the practical use of the geometric integration methods that were discussed.

All the chapters collect some exercises at the end. Some assumed knowledge is collected in appendices (differential equations, some numerical solution methods, and elements of a Lie agebra and Lie groups). An introduction to Hamiltonian systems is distributed over several chapters. Matlab implementations of the methods (i.e. the ones used to generate the figures of this book) are made available on the author's website.

This being an introduction, several topics were not discussed but a reference is given to look them up: e.g., multistep methods and the use of variable time steps, or energy preserving methods, constrained systems, high oscillation systems, Poisson systems, and Hamiltonian PDEs.

This second edition comes about 10 years after the first edition. The authors have rewritten Chapter 3 and extended several topics in the other chapters (non-autonomous systems, positivity preservation, a new Chapter 7 and new exercises are added, figures are improved, and the list of references extended).

This is a very good introduction to the subject for students, and researches in numerical analysis but also in the many fields of science and engineering where these methods are essential computational tools.

Reviewer: Adhemar Bultheel (Leuven)

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MSC:

Cited in **1** Document

65-02	Research exposition (monographs, survey articles) pertaining to numerical analysis
65P10	Numerical methods for Hamiltonian systems including symplectic integrators
65M06	Finite difference methods for initial value and initial-boundary value problems involving PDEs
65M70	Spectral, collocation and related methods for initial value and initial-boundary value problems involving PDEs
70F05	Two-body problems
70H05	Hamilton's equations
37M15	Discretization methods and integrators (symplectic, variational, geometric, etc.) for dynamical systems
65L07	Numerical investigation of stability of solutions to ordinary differential equations
65L60	Finite element, Rayleigh-Ritz, Galerkin and collocation methods for ordinary differential equations
35K20	Initial-boundary value problems for second-order parabolic equations
65L70	Error bounds for numerical methods for ordinary differential equations
35Q41	Time-dependent Schrödinger equations and Dirac equations

Keywords:

Hamiltonian system; symplectic integrator; Euler symplectic; Stoermer-Verlet scheme; Runge-Kutta symplectic; multistep method; composition method; splitting method; variational integrator; volume-preserving method; Lie group method; extrapolation method; linear parabolic PDE; monograph; backward error analysis; Schrödinger equation; finite differences; Fourier spectral collocation

Software:

Matlab; Simulink

Full Text: DOI

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