Structure-Preserving Algorithms for Oscillatory Differential Equations

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Preface

Effective numerical solution of differential equations, although as old as differential equations themselves, has been a great challenge to numerical analysts, scientists and engineers for centuries. In recent decades, it has been universally acknowledged that differential equations arising in science and engineering often have certain structures that require preservation by the numerical integrators. Beginning with the symplectic integration of R. de Vogelaere (1956), R.D. Ruth (1983), Feng Kang (1985), J.M. Sanz-Serna (1988), E. Hairer (1994) and others, structure-preserving computation, or geometric numerical integration, has become one of the central fields of numerical differential equations. Geometric numerical integration aims at the preservation of the physical or geometric features of the exact flow of the system in long-term computation, such as the symplectic structure of Hamiltonian systems, energy and momentum of dynamical systems, time-reversibility of conservative mechanical systems, oscillatory and high oscillatory systems.

The objective of this monograph is to study structure-preserving algorithms for oscillatory problems that arise in a wide range of fields such as astronomy, molecular dynamics, classical mechanics, quantum mechanics, chemistry, biology and engineering. Such problems can often be modeled by initial value problems of second-order differential equations with a linear term characterizing the oscillatory structure of the systems. Since general-purpose high order Runge–Kutta (RK) methods, Runge–Kutta–Nyström (RKN) methods, and linear multistep methods (LMM) cannot respect the special structures of oscillatory problems in long-term integration, innovative integrators have to be designed. This monograph systematically develops theories and methods for solving second-order differential equations with oscillatory solutions.

As the basis of the whole monograph, Chap. 1 reviews the general notions and ideas related to the numerical integration of oscillatory differential equations. Chapter 2 presents multidimensional RKN methods adapted to second-order oscillatory systems.

Chapter 3 proposes extended Runge–Kutta–Nyström (ERKN) methods for initial value problems of second-order oscillatory systems with a constant frequency matrix or with a variable frequency matrix. The scheme of ERKN methods incorporates the particular structure of the differential equations into both the internal stages and the updates. A tri-colored tree theory, namely, the special extended Nyström tree (SEN-tree) theory and the related B-series theory are established, based on which the order conditions for ERKN methods are derived. The relation between ERKN methods and exponentially fitted methods is investigated. Multidimensional ERKN methods and multidimensional exponentially fitted methods are constructed.

Chapter 4 focuses on ERKN methods for oscillatory Hamiltonian systems. The symplecticity and symmetry conditions for ERKN methods are presented. Symplectic and symmetric ERKN (SSERKN) methods are applied to the Fermi–Pasta–Ulam problem and some nonlinear wave equations such as the sine-Gordon equation.

The idea of ERKN methods is extended to two-step hybrid methods in Chap. 5, to Falkner-type methods in Chap. 6, to energy-preserving methods in Chap. 7, to asymptotic methods for highly oscillatory problems in Chap. 8, and to multi-symplectic methods for Hamiltonian partial differential equations in Chap. 9.

All the numerical integrators presented in this monograph have been tested for oscillatory problems from a variety of applications. They are shown to be more efficient than some existing high quality methods in the scientific literature.

Chapters 1 and 2 and Sect. 3.1 of Chap. 3 are more theoretical. Scientists and engineers who are mainly interested in numerical integrators may skip them, and this will not affect the comprehension of the rest of the monograph.

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