

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 incor-

porates the particular structure of the differential equations into both the internal stages and the updates. A tri-colored tree theory, namely, the special extended Nystrom 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 multisymplectic 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.

We are grateful to all the friends and colleagues for their selfless help during the preparation of this monograph. Special thanks are due to John Butcher of The University of Auckland, Christian Lubich of Universität Tübingen, Arieh Iserles of University of Cambridge, Jeff Cash of Imperial College London, Maarten de Hoop of Purdue University, Qin Sheng of Baylor University, Tobias Jahnke of Karlsruher Institut für Technologie (KIT), Achim Schädle of Heinrich Heine University Düsseldorf, Reinout Quispel and David McLaren of La Trobe University, Jesus Vigo-Aguiar of Universidad de Salamanca, and Richard Terrill of Minnesota State University for their encouragement.

We are also grateful to many friends and colleagues for reading the manuscript and for their valuable suggestions and discussions. In particular, we are grateful to Robert Peng Kong Chan of The University of Auckland, Weixing Zheng, Zuhe Shen of Nanjing University, Jianlin Xia of Purdue University, Adrian Turton Hill of Bath University, Jichun Li of University of Nevada, Las Vegas, and Xiaowen Chang of McGill University.

Thanks also go to the following people for their various help and support: Cheng Fang, Peiheng Wu, Rong Zhang, Cong Cong, Manchun Li, Shengwang Wang, Jipu Ma, Qiguang Wu, Xianglin Fei, Lin Liu, Yucheng Su, Xuesong Bao, Chengsen Lin, Wenting Tong, Chunhong Xie, Dongping Jiang, Zixiang Ouyang, Liangsheng Luo, Jinxi Zhao, Xinbao Ning, Weixue Shi, Chengkui Zhong, Jiangong You, Hourong Qin, Huicheng Yin, Xiaosheng Zhu, Zhiwei Sun, Qiang Zhang, Gaofei Zhang, Chun Li and Zhi Qian of Nanjing University, Yaolin Jiang of Xi'an Jiao Tong University, Yongzhong Song and Yushun Wang of Nanjing Normal University, Jialin Hong and Zaijiu Shang of Chinese Academy of Sciences, Jijun Liu and Zhizhong Sun of Southeast University, Shoufo Li and Aiguo Xiao of Xiang Tan University,

Chuanmiao Chen of Hunan Normal University, Siqing Gan of Central South University, Chengjian Zhang and Chengming Huang of Huazhong University of Science & Technology, Shuanghu Wang of the Institute of Applied Physics and Computational Mathematics, Beijing, Hongjiong Tian of Shanghai Normal University, Yongkui Zou of Jilin University, Jingjun Zhao of Harbin Institute of Technology, Qinghong Li of Chuzhou University, Yonglei Fang of Zaozhuang University, Fan Yang and Hongli Yang of Nanjing Institute of Technology, Jiyong Li of Hebei Normal University, Wei Shi, Kai Liu, Qihua Huang, Jun Wu, Jinsong Yu and Guozhong Hu.

We would like to thank Ji Luo for her help with the editing, the editorial and production group of the Science Press, Beijing, and Springer-Verlag, Heidelberg.

We also thank our families for their love and support throughout all these years.

The work on this monograph was supported in part by the Specialized Research Foundation for the Doctoral Program of Higher Education under Grant 20100091110033, by the 985 Project at Nanjing University under Grant 9112020301, by the Natural Science Foundation of China under Grant 10771099, Grant 11271186 and Grant 11171155, and by the Priority Academic Program Development of Jiangsu Higher Education Institutions.

Nanjing

Xinyuan Wu

Xiong You

Bin Wang

Structure-Preserving Algorithms for Oscillatory
Differential Equations

Wu, X.; You, X.; Wang, B.

2013, XII, 236 p. 40 illus., 2 illus. in color., Hardcover

ISBN: 978-3-642-35337-6