



Xinyuan Wu · Kai Liu
Wei Shi

Structure-Preserving Algorithms for Oscillatory Differential Equations II



Science Press
Beijing



Springer

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ISBN 978-3-662-48155-4 ISBN 978-3-662-48156-1 (eBook)
DOI 10.1007/978-3-662-48156-1

Jointly published with Science Press, Beijing, China
ISBN: 978-7-03-043918-5 Science Press, Beijing

Library of Congress Control Number: 2015950922

Springer Heidelberg New York Dordrecht London

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This monograph is dedicated to Prof. Kang Feng on the thirtieth anniversary of his pioneering study on symplectic algorithms.

His profound work, which opened up a rich new field of research, is of great importance to numerical mathematics in China, and the influence of his seminal contributions has spread throughout the world.



2014 Nanjing Workshop on Structure-Preserving Algorithms for Differential Equations (Nanjing, November 29, 2014)

Preface

Numerical integration of differential equations, as an essential tool for investigating the qualitative behaviour of the physical universe, is a very active research area since large-scale science and engineering problems are often modelled by systems of ordinary and partial differential equations, whose analytical solutions are usually unknown even when they exist. Structure preservation in numerical differential equations, known also as geometric numerical integration, has emerged in the last three decades as a central topic in numerical mathematics. It has been realized that an integrator should be designed to preserve as much as possible the (physical/geometric) intrinsic properties of the underlying problem. The design and analysis of numerical methods for oscillatory systems is an important problem that has received a great deal of attention in the last few years. We seek to explore new efficient classes of methods for such problems, that is high accuracy at low cost. The recent growth in the need of geometric numerical integrators has resulted in the development of numerical methods that can systematically incorporate the structure of the original problem into the numerical scheme. The objective of this sequel to our previous monograph, which was entitled “Structure-Preserving Algorithms for Oscillatory Differential Equations”, is to study further structure-preserving integrators for multi-frequency oscillatory systems that arise in a wide range of fields such as astronomy, molecular dynamics, classical and quantum mechanics, electrical engineering, electromagnetism and acoustics. In practical applications, such problems can often be modelled by initial value problems of second-order differential equations with a linear term characterizing the oscillatory structure. As a matter of fact, this extended volume is a continuation of the previous volume of our monograph and presents the latest research advances in structure-preserving algorithms for multi-frequency oscillatory second-order differential equations. Most of the materials of this new volume are drawn from very recent published research work in professional journals by the research group of the authors.

Chapter 1 analyses in detail the matrix-variation-of-constants formula which gives significant insight into the structure of the solution to the multi-frequency and multidimensional oscillatory problem. It is known that the Störmer–Verlet formula

is a very popular numerical method for solving differential equations. Chapter 2 presents novel improved multi-frequency and multidimensional Störmer–Verlet formulae. These methods are applied to solve four significant problems. For structure-preserving integrators in differential equations, another related area of increasing importance is the computation of highly oscillatory problems. Therefore, Chap. 3 explores improved Filon-type asymptotic methods for highly oscillatory differential equations. In recent years, various energy-preserving methods have been developed, such as the discrete gradient method and the average vector field (AVF) method. In Chap. 4, we consider efficient energy-preserving integrators based on the AVF method for multi-frequency oscillatory Hamiltonian systems. An extended discrete gradient formula for multi-frequency oscillatory Hamiltonian systems is introduced in Chap. 5. It is known that collocation methods for ordinary differential equations have a long history. Thus, in Chap. 6, we pay attention to trigonometric Fourier collocation methods with arbitrary degrees of accuracy in preserving some invariants for multi-frequency oscillatory second-order ordinary differential equations. Chapter 7 analyses the error bounds for explicit ERKN integrators for systems of multi-frequency oscillatory second-order differential equations. Chapter 8 contains an analysis of the error bounds for two-step extended Runge–Kutta–Nyström-type (TSERKN) methods. Symplecticity is an important characteristic property of Hamiltonian systems and it is worthwhile to investigate higher order symplectic methods. Therefore, in Chap. 9, we discuss high-accuracy explicit symplectic ERKN integrators. Chapter 10 is concerned with multi-frequency adapted Runge–Kutta–Nyström (ARKN) integrators for general multi-frequency and multidimensional oscillatory second-order initial value problems. Butcher’s theory of trees is widely used in the study of Runge–Kutta and Runge–Kutta–Nyström methods. Chapter 11 develops a simplified tricoloured tree theory for the order conditions for ERKN integrators and the results presented in this chapter are an important step towards an efficient theory of this class of schemes. Structure-preserving algorithms for multi-symplectic Hamiltonian PDEs are of great importance in numerical simulations. Chapter 12 focuses on general approach to deriving local energy-preserving integrators for multi-symplectic Hamiltonian PDEs.

The presentation of this volume is characterized by mathematical analysis, providing insight into questions of practical calculation, and illuminating numerical simulations. All the integrators presented in this monograph have been tested and verified on multi-frequency oscillatory problems from a variety of applications to observe the applicability of numerical simulations. They seem to be more efficient than the existing high-quality codes in the scientific literature.

The authors are grateful to all their friends and colleagues for their selfless help during the preparation of this monograph. Special thanks go to John Butcher of The University of Auckland, Christian Lubich of Universität Tübingen, Arieh Iserles of University of Cambridge, Reinout Quispel of La Trobe University, Jesus Maria Sanz-Serna of Universidad de Valladolid, Peter Eris Kloeden of Goethe–Universität, Elizabeth Louise Mansfield of University of Kent, Maarten de Hoop of Purdue University, Tobias Jahnke of Karlsruher Institut für Technologie (KIT),

Achim Schädle of Heinrich Heine University Düsseldorf and Jesus Vigo-Aguiar of Universidad de Salamanca for their encouragement.

The authors are also indebted to many friends and colleagues for reading the manuscript and for their valuable suggestions. In particular, the authors take this opportunity to express their sincere appreciation to Robert Peng Kong Chan of The University of Auckland, Qin Sheng of Baylor University, Jichun Li of University of Nevada Las Vegas, Adrian Turton Hill of Bath University, Choi-Hong Lai of University of Greenwich, Xiaowen Chang of McGill University, Jianlin Xia of Purdue University, David McLaren of La Trobe University, Weixing Zheng and Zuhe Shen of Nanjing University.

Sincere thanks also go to the following people for their help and support in various forms: Cheng Fang, Peiheng Wu, Jian Lü, Dafu Ji, Jinxi Zhao, Liangsheng Luo, Zhihua Zhou, Zehua Xu, Nanqing Ding, Guofei Zhou, Yiqian Wang, Jiansheng Geng, Weihua Huang, Jiangong You, Hourong Qin, Haijun Wu, Weibing Deng, Rong Shao, Jiaqiang Mei, Hairong Xu, Liangwen Liao and Qiang Zhang of Nanjing University, Yaolin Jiang of Xi'an Jiao Tong University, Yongzhong Song, Jinru Chen and Yushun Wang of Nanjing Normal University, Xinru Wang of Nanjing Medical University, Mengzhao Qin, Geng Sun, Jialin Hong, Zaijiu Shang and Yifa Tang of Chinese Academy of Sciences, Guangda Hu of University of Science and Technology Beijing, Jijun Liu, Zhizhong Sun and Hongwei Wu of Southeast University, Shoufo Li, Aiguo Xiao and Liping Wen 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 and Technology, Shuanghu Wang of the Institute of Applied Physics and Computational Mathematics, Beijing, Yuhao Cong of Shanghai University, Hongjiong Tian of Shanghai Normal University, Yongkui Zou of Jilin University, Jingjun Zhao of Harbin Institute of Technology, Qin Ni and Chunwu Wang of Nanjing University of Aeronautics and Astronautics, Guoqing Liu, and Hao Cheng of Nanjing Tech University, Hongyong Wang of Nanjing University of Finance and Economics, Theodoros Kouloukas of La Trobe University, Anders Christian Hansen, Amandeep Kaur and Virginia Mullins of University of Cambridge, Shixiao Wang of The University of Auckland, Qinghong Li of Chuzhou University, Yonglei Fang of Zaozhuang University, Fan Yang, Xianyang Zeng and Hongli Yang of Nanjing Institute of Technology, Jiyong Li of Hebei Normal University, Bin Wang of Qufu Normal University, Xiong You of Nanjing Agricultural University, Xin Niu of Hefei University, Hua Zhao of Beijing Institute of Tracking and Tele Communication Technology, Changying Liu, Lijie Mei, Yuwen Li, Qihua Huang, Jun Wu, Lei Wang, Jinsong Yu, Guohai Yang and Guozhong Hu.

The authors would like to thank Kai Hu, Ji Luo and Tianren Sun for their help with the editing, the editorial and production group of the Science Press, Beijing and Springer-Verlag, Heidelberg.

The authors also thank their family members for their love and support throughout all these years.

The work on this monograph was supported in part by the Natural Science Foundation of China under Grants 11271186, by NSFC and RS International Exchanges Project under Grant 113111162, by the Specialized Research Foundation for the Doctoral Program of Higher Education under Grant 20100091110033 and 20130091110041, by the 985 Project at Nanjing University under Grant 9112020301, and by the Priority Academic Program Development of Jiangsu Higher Education Institutions.

Nanjing, China

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Contents

1	Matrix-Variation-of-Constants Formula	1
1.1	Multi-frequency and Multidimensional Problems	1
1.2	Matrix-Variation-of-Constants Formula	3
1.3	Towards Classical Runge-Kutta-Nyström Schemes	8
1.4	Towards ARKN Schemes and ERKN Integrators	9
1.4.1	ARKN Schemes	9
1.4.2	ERKN Integrators	10
1.5	Towards Two-Step Multidimensional ERKN Methods	11
1.6	Towards AAVF Methods for Multi-frequency Oscillatory Hamiltonian Systems	13
1.7	Towards Filon-Type Methods for Multi-frequency Highly Oscillatory Systems	14
1.8	Towards ERKN Methods for General Second-Order Oscillatory Systems	16
1.9	Towards High-Order Explicit Schemes for Hamiltonian Nonlinear Wave Equations	17
1.10	Conclusions and Discussions	18
	References	20
2	Improved Störmer–Verlet Formulae with Applications	23
2.1	Motivation	23
2.2	Two Improved Störmer–Verlet Formulae	26
2.2.1	Improved Störmer–Verlet Formula 1	26
2.2.2	Improved Störmer–Verlet Formula 2	29
2.3	Stability and Phase Properties	31
2.4	Applications	33
2.4.1	Application 1: Time-Independent Schrödinger Equations	34
2.4.2	Application 2: Non-linear Wave Equations	35
2.4.3	Application 3: Orbital Problems	37
2.4.4	Application 4: Fermi–Pasta–Ulam Problem	40

2.5	Coupled Conditions for Explicit Symplectic and Symmetric Multi-frequency ERKN Integrators for Multi-frequency Oscillatory Hamiltonian Systems	42
2.5.1	Towards Coupled Conditions for Explicit Symplectic and Symmetric Multi-frequency ERKN Integrators	43
2.5.2	The Analysis of Combined Conditions for SSMERKN Integrators for Multi-frequency and Multidimensional Oscillatory Hamiltonian Systems	44
2.6	Conclusions and Discussions	48
	References.	49
3	Improved Filon-Type Asymptotic Methods for Highly Oscillatory Differential Equations	53
3.1	Motivation	53
3.2	Improved Filon-Type Asymptotic Methods.	54
3.2.1	Oscillatory Linear Systems.	56
3.2.2	Oscillatory Nonlinear Systems	59
3.3	Practical Methods and Numerical Experiments	61
3.4	Conclusions and Discussions	66
	References.	67
4	Efficient Energy-Preserving Integrators for Multi-frequency Oscillatory Hamiltonian Systems	69
4.1	Motivation	69
4.2	Preliminaries	71
4.3	The Derivation of the AAVF Formula	73
4.4	Some Properties of the AAVF Formula	77
4.4.1	Stability and Phase Properties	77
4.4.2	Other Properties	79
4.5	Some Integrators Based on AAVF Formula	83
4.6	Numerical Experiments	87
4.7	Conclusions	91
	References.	92
5	An Extended Discrete Gradient Formula for Multi-frequency Oscillatory Hamiltonian Systems	95
5.1	Motivation	95
5.2	Preliminaries	98
5.3	An Extended Discrete Gradient Formula Based on ERKN Integrators	100
5.4	Convergence of the Fixed-Point Iteration for the Implicit Scheme	104

5.5	Numerical Experiments	109
5.6	Conclusions	114
	References.	114
6	Trigonometric Fourier Collocation Methods for Multi-frequency Oscillatory Systems.	117
6.1	Motivation	117
6.2	Local Fourier Expansion	120
6.3	Formulation of TFC Methods	121
6.3.1	The Calculation of $I_{1,j}$, $I_{2,j}$	122
6.3.2	Discretization	124
6.3.3	The TFC Methods.	125
6.4	Properties of the TFC Methods.	128
6.4.1	The Order	129
6.4.2	The Order of Energy Preservation and Quadratic Invariant Preservation	130
6.4.3	Convergence Analysis of the Iteration	133
6.4.4	Stability and Phase Properties.	135
6.5	Numerical Experiments	137
6.6	Conclusions and Discussions	146
	References.	146
7	Error Bounds for Explicit ERKN Integrators for Multi-frequency Oscillatory Systems.	149
7.1	Motivation	149
7.2	Preliminaries for Explicit ERKN Integrators	150
7.2.1	Explicit ERKN Integrators and Order Conditions	152
7.2.2	Stability and Phase Properties.	154
7.3	Preliminary Error Analysis.	155
7.3.1	Three Elementary Assumptions and a Gronwall's Lemma.	155
7.3.2	Residuals of ERKN Integrators.	156
7.4	Error Bounds	159
7.5	An Explicit Third Order Integrator with Minimal Dispersion Error and Dissipation Error	166
7.6	Numerical Experiments	169
7.7	Conclusions	173
	References.	173
8	Error Analysis of Explicit TSERKN Methods for Highly Oscillatory Systems.	175
8.1	Motivation	175
8.2	The Formulation of the New Method.	176
8.3	Error Analysis	183

8.4	Stability and Phase Properties	186
8.5	Numerical Experiments	188
8.6	Conclusions	191
	References	192
9	Highly Accurate Explicit Symplectic ERKN Methods for Multi-frequency Oscillatory Hamiltonian Systems	193
9.1	Motivation	193
9.2	Preliminaries	194
9.3	Explicit Symplectic ERKN Methods of Order Five with Some Small Residuals	196
9.4	Numerical Experiments	204
9.5	Conclusions and Discussions	208
	References	208
10	Multidimensional ARKN Methods for General Multi-frequency Oscillatory Second-Order IVPs	211
10.1	Motivation	211
10.2	Multidimensional ARKN Methods and the Corresponding Order Conditions	212
10.3	ARKN Methods for General Multi-frequency and Multidimensional Oscillatory Systems	214
10.3.1	Construction of Multidimensional ARKN Methods	215
10.3.2	Stability and Phase Properties of Multidimensional ARKN Methods	220
10.4	Numerical Experiments	222
10.5	Conclusions and Discussions	225
	References	227
11	A Simplified Nyström-Tree Theory for ERKN Integrators Solving Oscillatory Systems	229
11.1	Motivation	229
11.2	ERKN Methods and Related Issues	231
11.3	Higher Order Derivatives of Vector-Valued Functions	233
11.3.1	Taylor Series of Vector-Valued Functions	233
11.3.2	Kronecker Inner Product	234
11.3.3	The Higher Order Derivatives and Kronecker Inner Product	235
11.3.4	A Definition Associated with the Elementary Differentials	236
11.4	The Set of Simplified Special Extended Nyström Trees	238
11.4.1	Tree Set SSENT and Related Mappings	238
11.4.2	The Set SSENT and the Set of Classical SN-Trees	242
11.4.3	The Set SSENT and the Set SENT	245

11.5	B-series and Order Conditions	246
11.5.1	B-series	247
11.5.2	Order Conditions	249
11.6	Conclusions and Discussions	251
	References.	252
12	General Local Energy-Preserving Integrators for Multi-symplectic Hamiltonian PDEs	255
12.1	Motivation	255
12.2	Multi-symplectic PDEs and Energy-Preserving Continuous Runge–Kutta Methods	256
12.3	Construction of Local Energy-Preserving Algorithms for Hamiltonian PDEs	258
12.3.1	Pseudospectral Spatial Discretization	258
12.3.2	Gauss-Legendre Collocation Spatial Discretization.	264
12.4	Local Energy-Preserving Schemes for Coupled Nonlinear Schrödinger Equations	268
12.5	Local Energy-Preserving Schemes for 2D Nonlinear Schrödinger Equations	272
12.6	Numerical Experiments for Coupled Nonlinear Schrödingers Equations.	275
12.7	Numerical Experiments for 2D Nonlinear Schrödinger Equations.	284
12.8	Conclusions	289
	References.	290
	Conference Photo (Appendix).	293
	Index	295

Chapter 1

Matrix-Variation-of-Constants Formula

The first chapter presents the matrix-variation-of-constants formula which is fundamental to structure-preserving integrators for multi-frequency and multidimensional oscillatory second-order differential equations in the current volume and the previous volume [23] of our monograph since the formula makes it possible to incorporate the special structure of the multi-frequency oscillatory problems into the integrators.

1.1 Multi-frequency and Multidimensional Problems

Oscillatory second-order initial value problems constitute an important category of differential equations in pure and applied mathematics, and in applied sciences such as mechanics, physics, astronomy, molecular dynamics and engineering. Among traditional and typical numerical schemes for solving these kinds of problems is the well-known Runge-Kutta-Nyström method [13], which has played an important role since 1925 in dealing with second-order initial value problems of the conventional form

$$\begin{cases} y'' = f(y, y'), & x \in [x_0, x_{\text{end}}], \\ y(x_0) = y_0, & y'(x_0) = y'_0. \end{cases} \quad (1.1)$$

However, many systems of second-order differential equations arising in applications have the general form

$$\begin{cases} y'' + My = f(y, y'), & x \in [x_0, x_{\text{end}}], \\ y(x_0) = y_0, & y'(x_0) = y'_0, \end{cases} \quad (1.2)$$

where $M \in \mathbb{R}^{d \times d}$ is a positive and semi-definite matrix (not necessarily diagonal nor symmetric, in general) that implicitly contains and preserves the main frequencies of the oscillatory problem. Here, $f : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}^d$, with the position $y(x) \in \mathbb{R}^d$ and

the velocity $y'(x)$ as arguments. The system (1.2) is a multi-frequency and multidimensional oscillatory problem which exhibits pronounced oscillatory behaviour due to the linear term My . Among practical examples we mention the damped harmonic oscillator, the van der Pol equation, the Liénard equation (see [10]) and the damped wave equation. The design and analysis of numerical integrators for nonlinear oscillators is an important problem that has received a great deal of attention in the last few years.

It is important to observe that the special case $M = \mathbf{0}$ in (1.2) reduces to the conventional form of second-order initial value problems (1.1). Therefore, each integrator for the system (1.2) is applicable to the conventional second-order initial value problems (1.1). Consequently, this extended volume of our monograph focuses only on the general second-order oscillatory system (1.2).

When the function f does not contain the first derivative y' , (1.2) reduces to the special and important multi-frequency oscillatory system

$$\begin{cases} y'' + My = f(y), & x \in [x_0, x_{\text{end}}], \\ y(x_0) = y_0, & y'(x_0) = y'_0. \end{cases} \quad (1.3)$$

If M is symmetric and positive semi-definite and $f(y) = -\nabla U(y)$, then with $q = y$, $p = y'$, (1.3) becomes identical to a multi-frequency and multidimensional oscillatory Hamiltonian system of the form

$$\begin{cases} p' = -\nabla_q H(p, q), & p(x_0) = p_0, \\ q' = \nabla_p H(p, q), & q(x_0) = q_0, \end{cases} \quad (1.4)$$

with the Hamiltonian

$$H(p, q) = \frac{1}{2} p^\top p + \frac{1}{2} q^\top M q + U(q), \quad (1.5)$$

where $U(q)$ is a smooth potential function. The solution of the system (1.4) exhibits nonlinear oscillations. Mechanical systems with a partitioned Hamiltonian function yield examples of this type. It is well known that two fundamental properties of Hamiltonian systems are:

- (i) the solutions preserve the Hamiltonian H , i.e., $H(p(x), q(x)) \equiv H(p_0, q_0)$ for any $x \geq x_0$;
- (ii) the corresponding flow is symplectic, i.e., it preserves the differential 2-form $\sum_{i=1}^d dp_i \wedge dq_i$.

It is true that great advances have been made in the theory of general-purpose methods for the numerical solution of ordinary differential equations. However, the numerical implementation of a general-purpose method cannot respect the qualitative behaviour of a multi-frequency and multidimensional oscillatory problem. It

turns out that structure-preserving integrators are required in order to produce the qualitative properties of the true flow of the multi-frequency oscillatory problem. This new volume represents an attempt to extend our previous volume [23] and presents the very recent advances in Runge-Kutta-Nyström-type (RKN-type) methods for multi-frequency oscillatory second-order initial value problems (1.2). To this end, the following matrix-variation-of-constants formula is fundamental and plays an important role.

1.2 Matrix-Variation-of-Constants Formula

The following matrix-variation-of-constants formula gives significant insight into the structure of the solution to the multi-frequency and multidimensional problem (1.2), which has motivated the formulation of multi-frequency and multidimensional adapted Runge-Kutta-Nyström (ARKN) schemes, and multi-frequency and multidimensional extended Runge-Kutta-Nyström (ERKN) integrators, as well as classical RKN methods.

Theorem 1.1 (Wu et al. [21]) *If $M \in \mathbb{R}^{d \times d}$ is a positive semi-definite matrix and $f : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}^d$ in (1.2) is continuous, then the exact solution of (1.2) and its derivative satisfy*

$$\begin{cases} y(x) = \phi_0((x - x_0)^2 M) y_0 + (x - x_0) \phi_1((x - x_0)^2 M) y'_0 \\ \quad + \int_{x_0}^x (x - \zeta) \phi_1((x - \zeta)^2 M) \hat{f}(\zeta) d\zeta, \\ y'(x) = -(x - x_0) M \phi_1((x - x_0)^2 M) y_0 + \phi_0((x - x_0)^2 M) y'_0 \\ \quad + \int_{x_0}^x \phi_0((x - \zeta)^2 M) \hat{f}(\zeta) d\zeta, \end{cases} \quad (1.6)$$

for $x_0, x \in (-\infty, +\infty)$, where

$$\hat{f}(\zeta) = f(y(\zeta), y'(\zeta))$$

and the matrix-valued functions $\phi_0(M)$ and $\phi_1(M)$ are defined by

$$\phi_0(M) = \sum_{k=0}^{\infty} \frac{(-1)^k M^k}{(2k)!}, \quad \phi_1(M) = \sum_{k=0}^{\infty} \frac{(-1)^k M^k}{(2k+1)!}. \quad (1.7)$$

We notice that these matrix-valued functions reduce to the ϕ -functions used for Gautschi-type trigonometric or exponential integrators in [4, 7] when M is a symmetric and positive semi-definite matrix.