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Structure-Preserving Algorithms for Oscillatory Differential Equations II

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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.

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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.

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Contents

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

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

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

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

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, $f : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$, with the position $y(x) \in \mathbb{R}^d$ and

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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

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

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

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

with the Hamiltonian

$$H(p, q) = \frac{1}{2}p^\intercal p + \frac{1}{2}q^\intercal Mq + U(q), \tag{1.5}$$

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 $\sum_{i=1}^{d} \mathrm{d}p_i \wedge \mathrm{d}q_i$.

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 $f : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$ in (1.2) is continuous, then the exact solution of (1.2) and its derivative satisfy*

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

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

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

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

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

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.