Journal of Computational and Applied Mathematics 263 (2014) 478–499

Contents lists available at ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

Special extended Nyström tree theory for ERKN methods

Xiong You[a,b,*], Yonglei Fang[c], Jinxi Zhao[b]

[a] *Department of Applied Mathematics, Nanjing Agricultural University, Nanjing 210095, PR China*
[b] *State Key Laboratory for Novel Software Technology, Nanjing University, Nanjing 210093, PR China*
[c] *Department of Mathematics and Information Science, Zaozhuang University, Zaozhuang 277160, PR China*

HIGHLIGHTS

- A systematic and uniform special extended Nyström tree (SEN-tree) theory.
- Order conditions for extended Runge–Kutta–Nyström (ERKN) methods.
- New simplifying assumptions for the coefficients of ERKN methods.
- Practical ERKN schemes with numerical illustrations.

ARTICLE INFO

Article history:
Received 22 August 2012
Received in revised form 17 September 2013

MSC:
primary 65L05
65L06
65M20
65N40
65R20

Keywords:
Special extended Nyström trees
Second-order oscillatory problems
Extended Runge–Kutta–Nyström methods
Order conditions

ABSTRACT

The aim of this paper is to develop a unified special extended Nyström tree (SEN-tree) theory which provides a theoretical framework for the order conditions of multidimensional extended Runge–Kutta–Nyström (ERKN) methods proposed by X. Wu et al. (Wu et al., 2010). The new SEN tree theory is complete and consistent, which has overcome the drawback of the bi-coloured tree theory in H. Yang et al.'s work (Yang et al., 2009) where two "branch sets" have to be constructed for the true solutions and for the numerical solutions, respectively.

1. Introduction

In recent years the effective numerical integration of the following the non-stiff second-order initial value problem (IVP)

$$\begin{cases} y'' + My = f(y), & t \in [x_0, x_{\text{end}}], \\ y(x_0) = y_0, & y'(x_0) = y_0', \end{cases} \tag{1}$$

has received great attention, where $y \in \mathbb{R}^d, f : \mathbb{R}^d \to \mathbb{R}^d$ is continuous, M is a $d \times d$ positive semi-definite coefficient matrix containing implicitly the frequencies of the problem. This type of problems arise naturally in a variety of areas such as

* Corresponding author at: Department of Applied Mathematics, Nanjing Agricultural University, Nanjing 210095, PR China.
E-mail addresses: youx@njau.edu.cn (X. You), ylfangmath@gmail.com (Y. Fang), jxzhao@nju.edu.cn (J. Zhao).

0377-0427/$ – see front matter © 2014 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.cam.2013.12.043

celestial mechanics, quantum physics, theoretical chemistry, electronics and so on. Before the work of Bettis [1], the problem (1) had been dealt with by the general-purpose Runge–Kutta (RK) methods, Runge–Kutta–Nyström (RKN) methods or linear multistep methods (LMM) (see [2–4]). Since these methods fail to take into account the special structure of the problem (1), they often give unsatisfactory numerical results.

In applications, it is often the case that the function $f(y)$ in (1) satisfies $f(y) = -\nabla U(y)$ for some smooth function $U(y)$. With the notation $q = y$ and $p = q'$, the system (1) is then a Hamiltonian system with the Hamiltonian

$$H(p, q) = \frac{1}{2}p^T p + \frac{1}{2}q^T Mq - U(q).$$

Symplectic RK or RKN methods have proved to preserve the symplectic structure of the exact flows of Hamiltonian systems in the long-run integration (see, for example, [3–6]). Among pioneers in symplectic methods we mention de Vogelaere [7], Ruth [8] and Feng [9,10]. Sanz-Serna [11], Hairer et al. [4] and Suris [12,13] have discovered the symplecticity conditions for RK methods, RKN and partitioned Runge–Kutta (PRK) methods, respectively. Order conditions for PRK and RKN methods are also derived via bi-coloured trees (i.e., Nyström trees) and the P-series theory in [4].

Bettis [1] is one of the first who consider the construction of the numerical integrators adapted to the oscillatory property of the solution to the problem (1). González et al. [14] give a family of explicit RK type methods for the system of the form (1) with $M = \omega^2 I_d$ ($\omega > 0$ is the principal frequency and I_d is the $d \times d$ identity matrix). When a good estimate of the frequency of the problem is known in advance, a new exponential fitting technique is invented to adapt the traditional methods to the oscillatory feature of the problem (1). See, for example, [15–22] for details. For second-order oscillatory differential equations, it is most natural to consider exponentially-fitted Runge–Kutta–Nyström (EFRKN) methods (see [23–25]). In particular, A. Tocino et al. [26] investigate the symplecticity conditions for exponentially fitted RKN methods. Very recently, Wu et al. [27] develop symplectic multidimensional exponentially fitted modified RKN methods for the system (1) as a Hamiltonian system.

On the other hand, Franco [28] modifies the updates of the traditional RKN methods and proposes the RKN methods adapted to perturbed oscillators (ARKN). Wu et al. [29] generalize Franco's one-dimensional version of ARKN methods to a multidimensional form. On the other hand, Yang et al. [30] observe that for the harmonic oscillator $y'' + \omega^2 y = 0$, the internal stages Y_i of an ARKN method fail to equal the exact values of the solution $y(x)$ at $t_n + c_i h$. Then they extend the characteristic form of the updates of ARKN methods to the internal stages and propose the extended Runge–Kutta–Nyström (ERKN) methods for the problem (1) in the case M is a diagonal matrix. Wu et al. [31] succeed forming the multidimensional ERKN methods for the more general problem (1). Chen et al. [32] construct symmetric and symplectic ERKN methods which outperform some highly efficient RKN type methods in the literature.

Compared with the traditional general form of the second-order problem $y'' = g(x, y)$, due to the special term $-My$ in the problem (1), the expansions of the true solutions and the numerical solutions have new terms characterized by the factor $-M$. Traditional (bi-coloured) Nyström tree (see [3]) are not adequate to represent these new elementary differentials. As a recipe, in the special case that M in the problem (1) is diagonal Yang et al. [30] develop a tri-coloured tree theory, from which the order conditions for ERKN methods are derived, based on which Wu et al. [31] derive the order conditions for multidimensional ERKN methods. However, this tree theory, consisting of a so-called *branch set* $\mathbb{BT}$ with some functions (order $\rho(\beta\tau)$, elementary differential $\mathcal{F}(\beta\tau)$, $\alpha(\beta\tau)$ and signed density $\gamma(\beta\tau)$) defined on the set, and a tree set $\mathbb{T}$ with corresponding functions, is complicated and is yet beautiful.

The purpose of this paper is to establish a new special extended Nyström tree (SEN-tree) theory with the aim at laying a theoretical foundation for the multidimensional ERKN methods proposed in [31]. We only need a set of bi-coloured trees (special extended Nystöm trees) *SENT*. All results on the expansion of the exact solution, the numerical solution and hence the order conditions are built up based on this set *SENT*. Here the matrix M in the system (1) is a general positive semi-definite matrix, even not necessarily symmetric. Thus the ERKN methods investigated in this paper are applicable to a wider range of second-order oscillatory problems. Another advantage of our ERKN methods is that the evaluation of matrix functions $\phi_0(V)$ and $\phi_1(V)$ and the other V-depend coefficients ($V = h^2 M$) in the scheme are free from the matrix decomposition of M and hence the cost of computation is largely reduced. In early work such as [14,15,17,24,25,28,33,34], they only deal with oscillatory systems with a single frequency. In [23], since w^2 is diagonal, $\phi_0(v), \phi_1(v), \bar{a}_{ij}(v), a_{ij}(v), \bar{b}_i(v),\ i, j = 1, 2, \ldots, s$ ($v = hw$) are all diagonal and their computation is essentially componentwise. The analysis and methods in [35] explicitly depend on the decomposition of the frequency matrix $M = \Omega^2$.

In Section 2, based on the matrix-valued ϕ-functions, a matrix form of the variation-of-constants formula is obtained, leading to the formulation of ERKN methods for the system (1). In Section 3 a new set of special extended Nyström trees (SEN-trees) are constructed to represent differentials in the expansions of higher derivatives of the true solutions of the system (1) and the numerical solutions produced by ERKN methods. Some important mappings are recursively defined on the SEN-tree set. Section 4 is concerned with the order conditions of ERKN methods derived by the new SEN tree theory. In Section 5 two explicit multidimensional ERKN integrators of respective orders four and five are derived from the order conditions and two simplifying conditions. In Section 6 we carry out some numerical experiments to illustrate the superiority of ERKN methods to several highly efficient codes in the literature. Section 7 is devoted to conclusions.