Numer Algor (2017) 75:909–935
DOI 10.1007/s11075-016-0225-5

ORIGINAL PAPER

An improved tri-coloured rooted-tree theory and order conditions for ERKN methods for general multi-frequency oscillatory systems

Xianyang Zeng[1,3] · **Hongli Yang**[1,2] · **Xinyuan Wu**[1,4]

Received: 4 June 2016 / Accepted: 14 October 2016 / Published online: 16 November 2016

Abstract This paper develops an improved tri-coloured rooted-tree theory for the order conditions for ERKN methods solving general multi-frequency and multi-dimensional second-order oscillatory systems. The bottleneck of the original tri-coloured rooted-tree theory is the existence of numerous redundant trees. In light of the fact that the sum of the products of the symmetries and the elementary differentials is meaningful, this paper naturally introduces the so-called extended elementary differential mappings. Then, the new improved tri-coloured rooted tree theory is established based on a subset of the original tri-coloured rooted-tree set. This new theory makes all redundant trees disappear, and thus, the order conditions of ERKN

✉ Xinyuan Wu
xywu@nju.edu.cn

Xianyang Zeng
zxy@njit.edu.cn

Hongli Yang
yanghongli1016@163.com

1 Department of Mathematics, Nanjing University, Nanjing, People's Republic of China

2 Industrial Center, Nanjing Institute of Technology, Nanjing, People's Republic of China

3 Department of Mathematics and Physics, Nanjing Institute of Technology, Nanjing, People's Republic of China

4 State Key Laboratory for Novel Software Technology at Nanjing University, Nanjing, People's Republic of China

methods for general multi-frequency and multidimensional second-order oscillatory systems are reduced greatly. Furthermore, with this new theory, we present some new ERKN methods of order up to four. Numerical experiments are implemented and the results show that ERKN methods can be competitive with other existing methods in the scientific literature, especially when comparatively large stepsizes are used.

Keywords Multi-frequency and multidimensional perturbed oscillators · General ERKN methods · Order conditions · B-series

Mathematics Subject Classification (2010) 65L05 · 65L06

1 Introduction

In this paper, we pay our attention to the rooted-tree theory and B-series for *extended Runge-Kutta-Nyström* (abbr. ERKN) methods solving general multi-frequency and multidimensional oscillatory second-order initial value problems (abbr. IVPs) of the form

$$\begin{cases} \boldsymbol{y}''(t) + M\boldsymbol{y}(t) = \boldsymbol{f}\left(\boldsymbol{y}(t), \boldsymbol{y}'(t)\right), & t \in [t_0, T], \\ \boldsymbol{y}(t_0) = \boldsymbol{y}_0, \quad \boldsymbol{y}'(t_0) = \boldsymbol{y}'_0, \end{cases} \tag{1}$$

where M is a $d \times d$ constant matrix implicitly containing the dominant frequencies of the system, $\boldsymbol{y} \in \mathbb{R}^d$,and $\boldsymbol{f} : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$, with the position $\boldsymbol{y}$ and the velocity $\boldsymbol{y}'$ as arguments. In the special case where the right-hand side of (1) does not depend on the velocity $\boldsymbol{y}'$, (1) reduces to the following special second-order oscillatory system

$$\begin{cases} \boldsymbol{y}''(t) + M\boldsymbol{y}(t) = \boldsymbol{f}\left(\boldsymbol{y}(t)\right), & t \in [t_0, T], \\ \boldsymbol{y}(t_0) = \boldsymbol{y}_0, \quad \boldsymbol{y}'(t_0) = \boldsymbol{y}'_0. \end{cases} \tag{2}$$

Furthermore, if M is symmetric and positive semi-definite and $\boldsymbol{f}(\boldsymbol{q}) = -\nabla \boldsymbol{U}(\boldsymbol{q})$, then, with $\boldsymbol{q} = \boldsymbol{y}$, $\boldsymbol{p} = \boldsymbol{y}'$, (2) becomes identical to a multi-frequency and multidimensional oscillatory Hamiltonian system

$$\begin{cases} \boldsymbol{p}' = -\nabla_{\boldsymbol{q}} H(\boldsymbol{p}, \boldsymbol{q}), & \boldsymbol{p}(x_0) = \boldsymbol{p}_0, \\ \boldsymbol{q}' = \nabla_{\boldsymbol{p}} H(\boldsymbol{p}, \boldsymbol{q}), & \boldsymbol{q}(x_0) = \boldsymbol{q}_0, \end{cases} \tag{3}$$

with the Hamiltonian

$$H(\boldsymbol{p}, \boldsymbol{q}) = \frac{1}{2}\boldsymbol{p}^{\intercal}\boldsymbol{p} + \frac{1}{2}\boldsymbol{q}^{\intercal}M\boldsymbol{q} + \boldsymbol{U}(\boldsymbol{q}), \tag{4}$$

where $\boldsymbol{U}(\boldsymbol{q})$ is a smooth potential function. For solving the multi-frequency and multi-dimensional oscillatory system (3), a large number of studies have been made (see e.g. [1–3]). The methods for problems (1) and (2) are especially important when M has large positive eigenvalues as in the case where the wave equations is semi-discretised in space (see e.g. [4–8]). Such problems arise in a wide range of fields such as astronomy, molecular dynamics, classical mechanics, quantum mechanics, chemistry, biology, and engineering.

ERKN methods were proposed originally in paper [9, 10] to solve the special oscillatory system (2). ERKN methods show their great charming in practical numerical simulation since they are specially designed to be adapted to the structure of the underlying oscillatory system and do not depend on the decomposition of the matrix M. ERKN methods have been widely investigated and used in numerous applications in the fields of science and engineering; for example, the idea of ERKN methods has been extended to two-step hybrid methods (see e.g. [11, 12]), to Falkner-type methods (see e.g. [13]), to Strömer-Verlet methods (see e.g. [14]), to energy-preserving methods (see e.g. [7, 15, 16]), and to symplectic and multi-symplectic methods (see e.g. [4, 17–19]). Meanwhile, the further research of ARKN methods, including the symplectic conditions and symmetry, has been conducted as well (see e.g. [20–24]).

In a recent paper [25], ERKN methods were extended to the general oscillatory system (1), and a tri-coloured tree theory called *extended Nyström tree theory* (abbr. EN-T theory) was analysed for the order conditions. Unfortunately, however, the EN-T theory is not completely satisfactory due to the existence of disastrous redundant trees. For example, there are seven redundant trees out of 16 trees for third order ERKN methods. In practice, in order to gain the order conditions for a specific ERKN method of order r, one has to draw all graphs first, and then select and delete about half of the redundant trees. It will be a great waste of time and effort. As a result, it is not convenient nor efficient for the use of the EN-T theory to achieve the order conditions for ERKN methods.

Hence, in this paper, we will present an improved theory to eliminate all these redundant trees. Similarly to what we have done for the special oscillatory system (2) in [26], *the extended elementary differentials* are required and will be analysed in detail.

This paper is organized as follows. We first summarize the ERKN method for the general oscillatory system (1) in Section 2, and then in Section 3, we illustrate that the EN-T theory proposed in [25] works weakly. In Section 4, we investigate *the set of improved extended-Nyström trees* and show the relations to some other tree sets in the literature. Section 5 focuses on the B-series associated with the ERKN method for the general oscillatory system (1), and Section 6 analyses the corresponding order conditions for the ERKN methods when applied to the general oscillatory system (1). In Section 7, we derive some ERKN methods of order up to four. The numerical experiments are made in Section 8. The last section is concerned with conclusions and discussions.

2 ERKN methods

To begin with, we summarize the following ERKN method using the matrix-variation-of-constants formula (see [10]) and quadrature formulae.

Definition 2.1 (See [25]) An s-stage extended Runge-Kutta-Nyström (abbr. ERKN) method for the numerical integration of the IVP (1) is defined by the following scheme

$$\begin{cases} Y_i = \phi_0(c_i^2 V)\boldsymbol{y}_n + c_i\phi_1(c_i^2 V)h\boldsymbol{y}_n' + h^2\sum_{j=1}^{s}\bar{a}_{ij}(V)\boldsymbol{f}(Y_j, Y_j'), \qquad i = 1,\ldots,s, \\ hY_i' = -c_i V\phi_1(c_i^2 V)\boldsymbol{y}_n + \phi_0(c_i^2 V)h\boldsymbol{y}_n' + h^2\sum_{j=1}^{s}a_{ij}(V)\boldsymbol{f}(Y_j, Y_j'), \quad i = 1,\ldots,s, \\ \boldsymbol{y}_{n+1} = \phi_0(V)\boldsymbol{y}_n + \phi_1(V)h\boldsymbol{y}_n' + h^2\sum_{i=1}^{s}\bar{b}_i(V)\boldsymbol{f}(Y_i, Y_i'), \\ h\boldsymbol{y}_{n+1}' = -V\phi_1(V)\boldsymbol{y}_n + \phi_0(V)h\boldsymbol{y}_n' + h^2\sum_{i=1}^{s}b_i(V)\boldsymbol{f}(Y_i, Y_i'), \end{cases} \tag{5}$$

where $\phi_0(V), \phi_1(V)$, $\bar{a}_{ij}(V)$, $a_{ij}(V)$, $\bar{b}_i(V)$, and $b_i(V)$ for $i, j = 1,\ldots,s$ are matrix-valued functions of $V = h^2M$, and are assumed to have the following series expansions

$$\bar{a}_{ij}(V) = \sum_{k=0}^{+\infty}\frac{\bar{a}_{ij}^{(2k)}}{(2k)!}V^k,\ a_{ij}(V) = \sum_{k=0}^{+\infty}\frac{a_{ij}^{(2k)}}{(2k)!}V^k,\ \bar{b}_i(V) = \sum_{k=0}^{+\infty}\frac{\bar{b}_i^{(2k)}}{(2k)!}V^k,$$

$$b_i(V) = \sum_{k=0}^{+\infty}\frac{b_i^{(2k)}}{(2k)!}V^k,\ \phi_i(V) = \sum_{k=0}^{+\infty}\frac{(-1)^k}{(2k+i)!}V^k$$

with real coefficients $\bar{a}_{ij}^{(2k)}, a_{ij}^{(2k)}, \bar{b}_i^{(2k)}, b_i^{(2k)}$ for $k = 0, 1, 2, \ldots$.

This ERKN method (5) in Definitions 2.1 can also be represented briefly in Butcher's tableau of coefficients [28]

$$\begin{array}{c|cccc|cccc} c_1 & \bar{a}_{11}(V) & \bar{a}_{12}(V) & \cdots & \bar{a}_{1s}(V) & a_{11}(V) & a_{12}(V) & \cdots & a_{1s}(V) \\ c_2 & \bar{a}_{21}(V) & \bar{a}_{22}(V) & \cdots & \bar{a}_{2s}(V) & a_{21}(V) & a_{22}(V) & \cdots & a_{2s}(V) \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & \bar{a}_{s1}(V) & \bar{a}_{s2}(V) & \cdots & \bar{a}_{ss}(V) & a_{s1}(V) & a_{s2}(V) & \cdots & a_{ss}(V) \\ \hline & \bar{b}_1(V) & \bar{b}_2(V) & \cdots & \bar{b}_s(V) & b_1(V) & b_2(V) & \cdots & b_s(V) \end{array} \tag{6}$$

In essence, ERKN methods incorporate the particular structure of the oscillatory system (1) into both the internal stages and the updates. Throughout this paper, we call methods for the general oscillatory system (1) as *general methods*, and *standard methods* for the special case (2).

3 The failure and the reduction of the EN-T theory

The EN-T theory for general ERKN methods was presented in the recent paper [25] in which some tri-coloured trees are supplemented to *the classical Nyström trees*

Table 1 Two EN-Ts which have the same elementary differentials $\mathcal{F}(\tau)(\boldsymbol{y}, \boldsymbol{y}')$

EN-Ts	ρ	γ	Φ_i	α	$\mathcal{F}$
	4	4	$c_i^2 \sum_j a_{ij}^{(0)}$	3	$\boldsymbol{f}^{(2)}_{\boldsymbol{y}\boldsymbol{y}'}(-M\boldsymbol{y}, \boldsymbol{f})$
	4	8	$c_i \sum_j \bar{a}_{ij}^{(0)}$	3	$\boldsymbol{f}^{(2)}_{\boldsymbol{y}\boldsymbol{y}'}(-M\boldsymbol{y}, \boldsymbol{f})$

(abbr. N-Ts). The idea of the EN-T theory comes from the fact that the numbers of the N-Ts and of the elementary differentials are completely different. The paper [25] tries to eliminate the difference and then to make one elementary differential corresponds to one tree uniquely. Unfortunately, however, the paper [25] cannot succeed in this point at all. For example, the two different trees shown in Table 1 have the same elementary differentials $\mathcal{F}(\tau)(\boldsymbol{y}, \boldsymbol{y}')$.

Moreover, the great limitation of the EN-T theory is the existence of great number of redundant trees that cause trouble in applications. For example, in Table 2 (left), there are seven EN-Ts but five of them are redundant since their order $\rho(\tau)$, density $\gamma(\tau)$, weight $\Phi_i(\tau)$, and the consequent order conditions can be implied by others for the general ERKN methods (5).

Here, it should be pointed out that one tree one elementary differential is not necessary. In other words, one tree may correspond to a set of elementary differentials. For example, just as shown in Table 2, the sum of the products of the symmetries $\alpha(\tau)$ and the elementary differentials $\mathcal{F}(\tau)(\boldsymbol{y}, \boldsymbol{y}')$ is meaningful. In fact, we have

$$\boldsymbol{f}^{(1)}_{\boldsymbol{y}}\boldsymbol{y}' + \boldsymbol{f}^{(1)}_{\boldsymbol{y}'}(-M\boldsymbol{y}) = D_h^1 \boldsymbol{f}\left(\phi_0(h^2M)\boldsymbol{y} + \phi_1(h^2M)h\boldsymbol{y}', \phi_0(h^2M)\boldsymbol{y}' - hM\phi_1(h^2M)\boldsymbol{y}\right),$$

Table 2 Some EN-Ts and the redundance

EN-Ts	ρ	γ	Φ_i	α	$\mathcal{F}$	EN-Ts	ρ	γ	Φ_i	α	$\mathcal{F}$
	2	2	c_i	1	$\boldsymbol{f}^{(1)}_{\boldsymbol{y}}\boldsymbol{y}'$		2	2	c_i	1	$\boldsymbol{f}^{(1)}_{\boldsymbol{y}}\boldsymbol{y}'$
	2	2	c_i	1	$\boldsymbol{f}^{(1)}_{\boldsymbol{y}'}(-M\boldsymbol{y})$						$+\boldsymbol{f}^{(1)}_{\boldsymbol{y}'}(-M\boldsymbol{y})$
	3	3	c_i^2	1	$\boldsymbol{f}^{(2)}_{\boldsymbol{y}\boldsymbol{y}}(\boldsymbol{y}', \boldsymbol{y}')$		3	3	c_i^2	1	$\boldsymbol{f}^{(2)}_{\boldsymbol{y}\boldsymbol{y}}(\boldsymbol{y}', \boldsymbol{y}')$
	3	3	c_i^2	2	$\boldsymbol{f}^{(2)}_{\boldsymbol{y}\boldsymbol{y}'}(-M\boldsymbol{y}, \boldsymbol{y}')$						$+2\boldsymbol{f}^{(2)}_{\boldsymbol{y}\boldsymbol{y}'}(-M\boldsymbol{y}, \boldsymbol{y}')$
	3	3	c_i^2	1	$\boldsymbol{f}^{(2)}_{\boldsymbol{y}'\boldsymbol{y}'}(-M\boldsymbol{y}, -M\boldsymbol{y})$						$+\boldsymbol{f}^{(2)}_{\boldsymbol{y}'\boldsymbol{y}'}(-M\boldsymbol{y}, -M\boldsymbol{y})$
	3	3	c_i^2	1	$\boldsymbol{f}^{(1)}_{\boldsymbol{y}}(-M\boldsymbol{y})$						$+\boldsymbol{f}^{(1)}_{\boldsymbol{y}}(-M\boldsymbol{y})$
	3	3	c_i^2	1	$\boldsymbol{f}^{(1)}_{\boldsymbol{y}'}(-M\boldsymbol{y}')$						$+\boldsymbol{f}^{(1)}_{\boldsymbol{y}'}(-M\boldsymbol{y}')$

namely, $\boldsymbol{f}^{(1)}_{\boldsymbol{y}}\boldsymbol{y}' + \boldsymbol{f}^{(1)}_{\boldsymbol{y}'}(-M\boldsymbol{y})$ is the first-order derivative of function $\boldsymbol{f}$ with respect to h, at $h = 0$, where the function $\boldsymbol{f}$ is evaluated at point $(\hat{\boldsymbol{y}}, \hat{\boldsymbol{y}}')$ with

$$\hat{\boldsymbol{y}} = \phi_0(h^2M)\boldsymbol{y} + \phi_1(h^2M)h\boldsymbol{y}', \tag{7}$$

$$\hat{\boldsymbol{y}}' = \phi_0(h^2M)\boldsymbol{y}' - hM\phi_1(h^2M)\boldsymbol{y}. \tag{8}$$

Thus, in Table 2, we can choose these two bi-coloured trees to represent the sums respectively and omit all trees with meagre vertices. In this way, we can get rid of redundance as shown in Table 2 (right).

On the other hand, although almost all tri-coloured trees are redundant, there indeed exist tri-coloured trees which are absolutely necessary in the research of order conditions for the general ERKN methods (5). For example, the fifth tree which is tri-coloured in the fifth line in the table 2 in [25] undoubtedly works in the order conditions. In a word, the theory for the general ERKN methods (5) is exactly a tri-coloured tree theory but it is on the basis of the subset of the EN-T set.

It is natural that this paper starts from the N-th derivative of the function $\boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m\boldsymbol{y}'^n}\Big|_{(\hat{\boldsymbol{y}},\hat{\boldsymbol{y}}')}$ with respect to h, at $h = 0$. For details about multivariate Taylor series expansions and some related knowledge, readers are referred to [26, 27]. In what follows, we will denote this derivative as $D^N_h\boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m\boldsymbol{y}'^n}$.

Remark 3.1 The dimension of the matrix $D^N_h\boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m\boldsymbol{y}'^n}$ is $d \times d^{m+n}$. If $\boldsymbol{z}$ is a $d^{m+n} \times 1$ matrix, the dimension of $D^N_h\boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m\boldsymbol{y}'^n}\boldsymbol{z}$ is $d \times 1$.

Remark 3.2 If the matrix M is null,

$$D^N_h\boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m\boldsymbol{y}'^n}\boldsymbol{z} = \boldsymbol{f}^{(m+n+N)}_{\boldsymbol{y}^{m+N}\boldsymbol{y}'^n}\left(\underbrace{\boldsymbol{y}', \cdots, \boldsymbol{y}'}_{N\text{ fold}}, \boldsymbol{z}\right),$$

where $\boldsymbol{f}^{(m+n+N)}_{\boldsymbol{y}^{m+N}\boldsymbol{y}'^n}$ is evaluated at the point $(\boldsymbol{y}, \boldsymbol{y}')$, and $(\cdot, \cdots, \cdot)$ is the Kronecker inner product (see [26]).

Remark 3.3 In the special case (2) where the function $\boldsymbol{f}$ is independent of $\boldsymbol{y}'$, $D^N_h\boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m\boldsymbol{y}'^n}\boldsymbol{z}$ is exactly $D^N_h\boldsymbol{f}^{(m)}\boldsymbol{z}$ in [26].

In the end of this section, we give the following first three results of $D^N_h\boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m\boldsymbol{y}'^n}\boldsymbol{z}$, which work significantly in the understanding of the extended elementary differentials (see Definition 4.2 in Section 4).

$$\begin{aligned}
D^1_h\boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m\boldsymbol{y}'^n}\boldsymbol{z} &= \boldsymbol{f}^{(m+n+1)}_{\boldsymbol{y}^{m+1}\boldsymbol{y}'^n}\left(\boldsymbol{y}', \boldsymbol{z}\right) + \boldsymbol{f}^{(m+n+1)}_{\boldsymbol{y}^m\boldsymbol{y}'^{n+1}}\left(-M\boldsymbol{y}, \boldsymbol{z}\right),\\
D^2_h\boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m\boldsymbol{y}'^n}\boldsymbol{z} &= \boldsymbol{f}^{(m+n+2)}_{\boldsymbol{y}^{m+2}\boldsymbol{y}'^n}\left(\boldsymbol{y}', \boldsymbol{y}', \boldsymbol{z}\right) + \boldsymbol{f}^{(m+n+1)}_{\boldsymbol{y}^{m+1}\boldsymbol{y}'^n}\left(-M\boldsymbol{y}, \boldsymbol{z}\right) + 2\boldsymbol{f}^{(m+n+2)}_{\boldsymbol{y}^{m+1}\boldsymbol{y}'^{n+1}}\left(\boldsymbol{y}', -M\boldsymbol{y}, \boldsymbol{z}\right)\\
&\quad + \boldsymbol{f}^{(m+n+2)}_{\boldsymbol{y}^m\boldsymbol{y}'^{n+2}}\left(-M\boldsymbol{y}, -M\boldsymbol{y}, \boldsymbol{z}\right) + \boldsymbol{f}^{(m+n+1)}_{\boldsymbol{y}^m\boldsymbol{y}'^{n+1}}\left(-M\boldsymbol{y}', \boldsymbol{z}\right),
\end{aligned}$$

$$
\begin{aligned}
D_h^3 \boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m \boldsymbol{y}'^n} \boldsymbol{z} = {} & \boldsymbol{f}^{(m+n+3)}_{\boldsymbol{y}^{m+3} \boldsymbol{y}'^n} \left(\boldsymbol{y}', \boldsymbol{y}', \boldsymbol{y}', \boldsymbol{z}\right) + 3\boldsymbol{f}^{(m+n+3)}_{\boldsymbol{y}^{m+2} \boldsymbol{y}'^{n+1}} \left(\boldsymbol{y}', \boldsymbol{y}', -M\boldsymbol{y}, \boldsymbol{z}\right) \\
& +3\boldsymbol{f}^{(m+n+3)}_{\boldsymbol{y}^{m+1} \boldsymbol{y}'^{n+2}} \left(\boldsymbol{y}', -M\boldsymbol{y}, -M\boldsymbol{y}, \boldsymbol{z}\right) \\
& +\boldsymbol{f}^{(m+n+3)}_{\boldsymbol{y}^{m} \boldsymbol{y}'^{n+3}} \left(-M\boldsymbol{y}, -M\boldsymbol{y}, -M\boldsymbol{y}, \boldsymbol{z}\right) + 3\boldsymbol{f}^{(m+n+2)}_{\boldsymbol{y}^{m+2} \boldsymbol{y}'^{n}} \left(\boldsymbol{y}', -M\boldsymbol{y}, \boldsymbol{z}\right) \\
& +3\boldsymbol{f}^{(m+n+2)}_{\boldsymbol{y}^{m+1} \boldsymbol{y}'^{n+1}} \left(-M\boldsymbol{y}, -M\boldsymbol{y}, \boldsymbol{z}\right) \\
& +3\boldsymbol{f}^{(m+n+2)}_{\boldsymbol{y}^{m+1} \boldsymbol{y}'^{n+1}} \left(\boldsymbol{y}', -M\boldsymbol{y}', \boldsymbol{z}\right) + 3\boldsymbol{f}^{(m+n+2)}_{\boldsymbol{y}^{m} \boldsymbol{y}'^{n+2}} \left(-M\boldsymbol{y}, -M\boldsymbol{y}', \boldsymbol{z}\right) \\
& +\boldsymbol{f}^{(m+n+1)}_{\boldsymbol{y}^{m+1} \boldsymbol{y}'^{n}} \left(-M\boldsymbol{y}', \boldsymbol{z}\right) + \boldsymbol{f}^{(m+n+1)}_{\boldsymbol{y}^{m} \boldsymbol{y}'^{n+1}} \left((-M)^2\boldsymbol{y}, \boldsymbol{z}\right).
\end{aligned}
$$

4 The set of improved extended-Nyström trees

In the study of order conditions for second order differential equations, there are four theory systems listed in Table 3, where the abbreviation "SSEN-T" comes from the expression of *simplified special extended Nyström-tree* [26], and here the word "compact" should be interpreted as that any order condition derived by a tree from the underlining rooted tree set cannot be obtained by others from the same rooted tree set.

The first two theory systems are much famous in the numerical analysis for ODEs, where the second is the special case of the first one. The rooted tree sets in these two theory systems are all bi-coloured tree sets with the white vertex and the black vertex. The last two theory systems are constructed on tri-coloured rooted tree sets by adding the meagre vertex to the graph of bi-coloured trees. Similarly, the last system is the special case of the third.

Moreover, when the matrix M is null, the third theory is identity to the first theory, and the fourth is the second. In a word, the last two theory systems are the extensions of the first two theory systems respectively. However, the extension of the first theory system is not satisfied yet, since the last section in this paper states that the third theory system is not compact. In order to make the extension better, a compact theory will be built to replace the third one, by introducing a completely new tri-coloured rooted tree set and six mappings on it. In this section, we will define the new tree set and study the relationships with the N-T set, the EN-T set and the SSEN-T set.

Table 3 Four theory systems for second order differential equations

	IVPs	Methods	Trees (graphs)	Compact (T/F)
1	$\boldsymbol{y}'' = \boldsymbol{f}\left(\boldsymbol{y}, \boldsymbol{y}'\right)$	General RKN methods	N-Ts	T
2	$\boldsymbol{y}'' = \boldsymbol{f}\left(\boldsymbol{y}\right)$	Standard RKN methods	SN-Ts	T
3	$\boldsymbol{y}'' + M\boldsymbol{y} = \boldsymbol{f}\left(\boldsymbol{y}, \boldsymbol{y}'\right)$	General ERKN methods	EN-Ts	F
4	$\boldsymbol{y}'' + M\boldsymbol{y} = \boldsymbol{f}\left(\boldsymbol{y}\right)$	Standard ERKN methods	SSEN-Ts	T

4.1 The IEN-T set and the related mappings

In this subsection, we will recursively define a new set named *the improved extended-Nyström tree set* and define six mappings on it.

Definition 4.1 The improved extended-Nyström tree (abbr. IEN-T) set is recursively defined as follows:

(a) $\circ$,  belong to the IEN-T set.
(b) If τ belongs to the IEN-T set, then the graph obtained by grafting the root of tree τ to a new black fat node and then to a new meagre node, $\cdots$ (p times), and then to a new black fat node and then last to a new white node, denoted by $W_+B_+(b_+B_+)^p(\tau)$ (see Table 4), belongs to the IEN-T set for $\forall p = 0, 1, 2, \ldots$.
(c) If τ belongs to the IEN-T set, then the graph obtained by grafting the root of tree τ to a new black fat node and then to a new meagre node, $\cdots$ (p times), then last to a new white node, denoted by $W_+(b_+B_+)^p(\tau)$ (see Table 4) belongs to the IEN-T set for $\forall p = 0, 1, 2, \ldots$.
(d) If $\tau_1, \cdots, \tau_\mu$ belong to the IEN-T set, then $\tau_1 \times \cdots \times \tau_\mu$ belongs to the IEN-T set, where "$\times$"' is the merging product [28].

Each tree τ in the IEN-T set can be denoted by

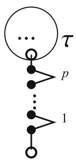
$$\tau := \underbrace{\tau_* \times \cdots \times \tau_*}_{N-\text{fold}} \times \left(W_+B_+(b_+B_+)^{p_1}(\tau_1)\right) \times \cdots \times \left(W_+B_+(b_+B_+)^{p_m}(\tau_m)\right)$$
$$\times \left(W_+(b_+B_+)^{q_1}(\tau_{m+1})\right) \times \cdots \times \left(W_+(b_+B_+)^{q_n}(\tau_{m+n})\right), \tag{9}$$

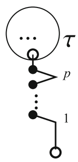
where $\tau_* =$ . Figure 1 gives the mode of the trees in the IEN-T set.

From Definition 4.1, the following rules for forming a tree τ in the IEN-T set can be obtained straightforwardly:

(i) The root of a tree is always a fat white vertex.
(ii) A white vertex has fat black children, or white children, or meagre children.
(iii) A fat black vertex has at most one child which can be white or meagre child.
(iv) A meagre vertex must have one fat black vertex as its child and must have a white vertex as its descendant.

Table 4 Tree $W_+B_+(b_+B_+)^p(\tau)$ (left) and tree $W_+(b_+B_+)^p(\tau)$ (right) in Definition 4.1





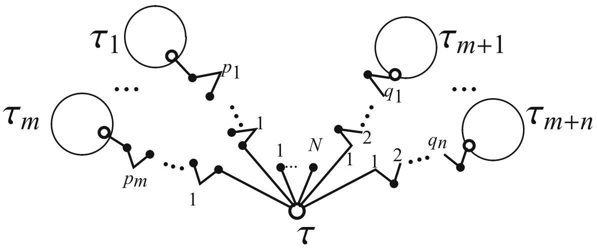


Fig. 1 The mode of the trees in the IEN-T set

Definition 4.2 The order $\rho(\tau)$, the extended elementary differential $\mathcal{F}(\tau)(\boldsymbol{y}, \boldsymbol{y}')$, the symmetry $\alpha(\tau)$, the weight $\Phi_i(\tau)$, the density $\gamma(\tau)$, and the sign $S(\tau)$ on the IEN-T set are recursively defined as follows.

1. $\rho(\circ) = 1$, $\mathcal{F}(\circ) = \boldsymbol{f}$, $\alpha(\circ) = 1$, $\Phi_i(\circ) = 1$, $\gamma(\circ) = 1$ and $S(\circ) = 1$.
2. For $\tau \in$ IEN-T denoted by (9),

- $\rho(\tau) = 1 + N + \sum_{i=1}^{m}(1 + 2p_i + \rho(\tau_i)) + \sum_{i=1}^{n}(2q_i + \rho(\tau_{m+i}))$,
- $\mathcal{F}(\tau) = D_h^N \boldsymbol{f}_{\boldsymbol{y}^m \boldsymbol{y}'^n}^{(m+n)}((-M)^{p_1}\mathcal{F}(\tau_1), \cdots, (-M)^{p_{m+n}}\mathcal{F}(\tau_{m+n}))$, where $p_{m+i} = q_i$, $i = 1, \cdots, n$, and $(\cdot, \cdots, \cdot)$ is the Kronecker inner product (see [26]),
- $\alpha(\tau) = (\rho(\tau) - 1)! \cdot \dfrac{1}{N!} \cdot \prod_{i=1}^{m}\left(\dfrac{\alpha(\tau_i)}{(1 + 2p_i + \rho(\tau_i))!}\right) \cdot \prod_{i=1}^{n}\left(\dfrac{\alpha(\tau_{m+i})}{(2q_i + \rho(\tau_{m+i}))!}\right) \cdot \dfrac{1}{J_1! \ldots J_I!}$, where $J_1, \cdots, J_I$ count the same branches,
- $\Phi_i(\tau) = c_i^N \cdot \prod_{k=1}^{m}\left(\sum_{j=1}^{s}\bar{a}_{ij}^{(2p_k)}\Phi_j(\tau_k)\right) \cdot \prod_{k=1}^{n}\left(\sum_{j=1}^{s}a_{ij}^{(2q_k)}\Phi_j(\tau_{m+k})\right)$,
- $\gamma(\tau) = \rho(\tau) \cdot \prod_{i=1}^{m}\left(\dfrac{(1 + 2p_i + \rho(\tau_i))!\gamma(\tau_i)}{(2p_i)!\rho(\tau_i)!}\right) \cdot \prod_{i=1}^{n}\left(\dfrac{(2q_i + \rho(\tau_{m+i}))!\gamma(\tau_{m+i})}{(2q_i)!\rho(\tau_{m+i})!}\right)$,
- $S(\tau) = \prod_{i=1}^{m}\left((-1)^{p_i}S(\tau_i)\right) \cdot \prod_{i=1}^{n}\left((-1)^{q_i}S(\tau_{m+i})\right)$,

where $\sum_{k=1}^{0} = 0$ and $\prod_{k=1}^{0} = 1$.

Definition 4.3 The set IEN-T$_m$ is defined as

$$\text{IEN-T}_m = \{\tau :\ \rho(\tau) = m,\ \tau \in \text{IEN-T}\}.$$

Remark 4.1 The order $\rho(\tau)$ is the number of the tree τ's vertices.

Remark 4.2 The extended elementary differential $\mathcal{F}(\tau)$ is a product of $(-M)^p$ (p is the number of meagre vertices between a white vertex and the next coming white vertex), and $D_h^N \boldsymbol{f}_{y^m y'^n}^{(n+m)}$ (N is the number of end vertices from the white vertex, m is the number of the non-ending black vertices from the white vertex, and n is the number of the meagre vertices from the white vertex). We will see that the extended elementary differential is not only one function but a weighted sum of the traditional elementary differential.

Remark 4.3 One IEN-T corresponds to one extended elementary differential $\mathcal{F}(\tau)$.

Remark 4.4 The symmetry $\alpha(\tau)$ is the number of possible different monotonic labeling of τ.

Remark 4.5 The weight $\Phi_i(\tau)$ is a sum over the indices of all white vertices and of all end vertices. The general term of the sum is a product of $\bar{a}_{ij}^{(2p)}$ for $W_+B_+(b_+B_+)^p(\tau)$, of $a_{ij}^{(2p)}$ for $W_+(b_+B_+)^p(\tau)$ (p is the number of the meagre vertices between the white vertices i and j) and of c_i^m (m is the number of end vertices from the white vertex i).

Remark 4.6 One IEN-T corresponds to one weight $\Phi_i(\tau)$.

Remark 4.7 The density $\gamma(\tau)$ is a product of the density of a tree by overlooking the differences between vertices and of $\frac{1}{(2p)!}$ (p is the number of the meagre vertices between two white vertices).

Remark 4.8 The sign $S(\tau)$ is 1 if the number of the meagre vertices is even, and -1 if the number of the meagre vertices is odd.

Table 5 presents the corresponding mappings: the order ρ, the sign S, the density γ, the weight Φ_i, the symmetry α, and the extended elementary differential $\mathcal{F}$ for each τ in the IEN-T set of order up to four.

4.2 The IEN-T set and the N-T set

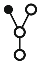
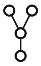
In this subsection, we can see that with the disappearance of meagre vertices the IEN-T set is exactly the N-T set. In fact, in this case, each tree τ in the IEN-T set has the mode shown in Fig. 2, and the rules to form the tree set are straightforwardly reduced to:

(i) The root of a tree is always a fat white vertex.

Table 5 IEN-Ts and mappings of order up to four and the corresponding elementary differentials on the N-T set

No.	IEN-Ts	ρ	S	γ	Φ_i	α	$\mathcal{F}$	$\mathcal{F}$ on the N-T set
1		1	1	1	1	1	$\boldsymbol{f}$	f
2		2	1	2	c_i	1	$D_h^1\boldsymbol{f}$	$f'_y y'$
3		2	1	2	$\sum_j a_{ij}^{(0)}$	1	$\boldsymbol{f}_{\boldsymbol{y}'}^{(1)}\boldsymbol{f}$	$f'_{y'} f$
4		3	1	3	c_i^2	1	$D_h^2\boldsymbol{f}$	$f''_{yy}(y', y')$
5		3	1	3	$c_i \sum_j a_{ij}^{(0)}$	1	$D_h^1\boldsymbol{f}_{\boldsymbol{y}'}\boldsymbol{f}$	$f''_{yy'}(y', f)$
6		3	1	3	$\sum_{j,k} a_{ij}^{(0)} a_{ik}^{(0)}$	1	$\boldsymbol{f}_{\boldsymbol{y}'\boldsymbol{y}'}(\boldsymbol{f}, \boldsymbol{f})$	$f''_{y'y'}(f, f)$
7		3	1	6	$\sum_j \bar{a}_{ij}^{(0)}$	1	$\boldsymbol{f}_{\boldsymbol{y}}^{(1)}\boldsymbol{f}$	$f'_y f$
8		3	1	6	$\sum_j a_{ij}^{(0)} c_j$	1	$\boldsymbol{f}_{\boldsymbol{y}'}^{(1)} D_h^1\boldsymbol{f}$	$f'_{y'} f_y y'$
9		3	1	6	$\sum_{j,k} a_{ij}^{(0)} a_{jk}^{(0)}$	1	$\boldsymbol{f}_{\boldsymbol{y}'}^{(1)}\boldsymbol{f}_{\boldsymbol{y}'}^{(1)}\boldsymbol{f}$	$f'_{y'} f'_{y'} f$
10		4	1	4	c_i^3	1	$D_h^3\boldsymbol{f}$	$f_{yyy}^{(3)}(y', y', y')$
11		4	1	4	$c_i^2 \sum_j a_{ij}^{(0)}$	3	$D_h^2\boldsymbol{f}_{\boldsymbol{y}'}^{(1)}\boldsymbol{f}$	$f_{y'yy}^{(3)}(f, y', y')$
12		4	1	4	$c_i \sum_{j,k} a_{ij}^{(0)} a_{ik}^{(0)}$	3	$D_h^1\boldsymbol{f}_{\boldsymbol{y}'\boldsymbol{y}'}^{(2)}(\boldsymbol{f}, \boldsymbol{f})$	$f_{yy'y'}^{(3)}(y', f, f)$
13		4	1	4	$\sum_{j,k,l} a_{ij}^{(0)} a_{ik}^{(0)} a_{il}^{(0)}$	1	$\boldsymbol{f}_{\boldsymbol{y}'\boldsymbol{y}'\boldsymbol{y}'}^{(3)}(\boldsymbol{f}, \boldsymbol{f}, \boldsymbol{f})$	$f_{y'y'y'}^{(3)}(f, f, f)$
14		4	1	8	$c_i \sum_j \bar{a}_{ij}^{(0)}$	3	$D_h^1\boldsymbol{f}_{\boldsymbol{y}}^{(1)}\boldsymbol{f}$	$f''_{yy}(y', f)$
15		4	1	8	$\sum_{j,k} \bar{a}_{ij}^{(0)} a_{ik}^{(0)}$	3	$\boldsymbol{f}_{\boldsymbol{y}\boldsymbol{y}'}^{(2)}(\boldsymbol{f}, \boldsymbol{f})$	$f''_{yy'}(f, f)$
16		4	1	8	$c_i \sum_{j,k} a_{ij}^{(0)} a_{jk}^{(0)}$	3	$D_h^1\boldsymbol{f}_{\boldsymbol{y}'}^{(1)}\boldsymbol{f}_{\boldsymbol{y}'}\boldsymbol{f}$	$f''_{yy'}(y', f_{y'} f)$
17		4	1	8	$\sum_{j,k,l} a_{ij}^{(0)} a_{ik}^{(0)} a_{kl}^{(0)}$	3	$\boldsymbol{f}_{\boldsymbol{y}'\boldsymbol{y}'}^{(2)}(\boldsymbol{f}, \boldsymbol{f}_{\boldsymbol{y}'}^{(1)}\boldsymbol{f})$	$f''_{y'y'}(f_{y'} f, f)$
18		4	1	8	$c_i \sum_j a_{ij}^{(0)} c_j$	3	$D_h^1\boldsymbol{f}_{\boldsymbol{y}'}^{(1)} D_h^1\boldsymbol{f}$	$f''_{yy'}(f_y y', y')$
19		4	1	8	$\sum_{j,k} a_{ij}^{(0)} a_{ik}^{(0)} c_k$	3	$\boldsymbol{f}_{\boldsymbol{y}'\boldsymbol{y}'}^{(2)}(\boldsymbol{f}, D_h^1\boldsymbol{f})$	$f''_{y'y'}(f_y y', f)$
20		4	1	24	$\sum_j \bar{a}_{ij}^{(0)} c_j$	1	$\boldsymbol{f}_{\boldsymbol{y}}^{(1)} D_h^1\boldsymbol{f}$	$f'_y f'_y y'$
21		4	1	24	$\sum_{j,k} \bar{a}_{ij}^{(0)} a_{jk}^{(0)}$	1	$\boldsymbol{f}_{\boldsymbol{y}}^{(1)}\boldsymbol{f}_{\boldsymbol{y}'}^{(1)}\boldsymbol{f}$	$f'_y f'_{y'} f$
22		4	1	24	$\sum_{j,k} a_{ij}^{(0)} \bar{a}_{jk}^{(0)}$	1	$\boldsymbol{f}_{\boldsymbol{y}'}^{(1)}\boldsymbol{f}_{\boldsymbol{y}}^{(1)}\boldsymbol{f}$	$f'_{y'} f'_y f$

Table 5 (continued)

No.	IEN-Ts	ρ	S	γ	Φ_i	α	$\mathcal{F}$	$\mathcal{F}$ on the N-T set
23		4	1	24	$\sum_{j,k} a_{ij}^{(0)} a_{jk}^{(0)} c_k$	1	$\boldsymbol{f}_{\boldsymbol{y}'}^{(1)} \boldsymbol{f}_{\boldsymbol{y}'}^{(1)} D_h^1 \boldsymbol{f}$	$f'_{y'} f'_{y'} f'_y y'$
24		4	1	24	$\sum_{j,k,l} a_{ij}^{(0)} a_{jk}^{(0)} a_{kl}^{(0)}$	1	$\boldsymbol{f}_{\boldsymbol{y}'}^{(1)} \boldsymbol{f}_{\boldsymbol{y}'}^{(1)} \boldsymbol{f}_{\boldsymbol{y}'}^{(1)} \boldsymbol{f}$	$f'_{y'} f'_{y'} f'_{y'} f$
25		4	-1	12	$\sum_j a_{ij}^{(2)}$	1	$\boldsymbol{f}_{\boldsymbol{y}'}^{(1)} (-M) \boldsymbol{f}$	–
26		4	1	12	$\sum_j a_{ij}^{(0)} c_j^2$	1	$\boldsymbol{f}_{\boldsymbol{y}'}^{(1)} D_h^2 \boldsymbol{f}$	$f'_{y'} f''_{yy}(y', y')$
27		4	1	12	$\sum_{j,k} a_{ij}^{(0)} c_j a_{jk}^{(0)}$	2	$\boldsymbol{f}_{\boldsymbol{y}'}^{(1)} D_h^1 \boldsymbol{f}_{\boldsymbol{y}'}^{(1)} \boldsymbol{f}$	$f'_{y'} f''_{yy'}(y', f)$
28		4	1	12	$\sum_{j,k,l} a_{ij}^{(0)} a_{jk}^{(0)} a_{jl}^{(0)}$	1	$\boldsymbol{f}_{\boldsymbol{y}'}^{(1)} \boldsymbol{f}_{\boldsymbol{y}'\boldsymbol{y}'}^{(2)} (\boldsymbol{f}, \boldsymbol{f})$	$f'_{y'} f''_{y'y'}(f, f)$

(ii) A white vertex has fat black children or white children.
(iii) A fat black vertex has at most one child which must be white.

In this case, from Remark 4.1 to Remark 4.7, the order $\rho(\tau)$, the symmetry $\alpha(\tau)$ and the density $\gamma(\tau)$ are exactly the same as the ones on the N-T set respectively. If M is null, the weight $\Phi_i(\tau)$ and the extended elementary differential $\mathcal{F}(\tau)(\boldsymbol{y}, \boldsymbol{y}')$ on the IEN-T set are exactly the same as the ones on the N-T set respectively, too. In fact, from Definition 4.2, with the disappearing of meagre vertices, these two mappings are recursively defined respectively, for τ denoted by Fig. 2, as follows:

$$\begin{aligned}
\Phi_i(\tau) &= c_i^N \cdot \prod_{k=1}^{m} \left(\sum_{j=1}^{s} \bar{a}_{ij} \Phi_j(\tau_k) \right) \cdot \prod_{k=1}^{n} \left(\sum_{j=1}^{s} a_{ij} \Phi_j(\tau_{m+k}) \right), \\
\mathcal{F}(\tau) &= D_h^N \boldsymbol{f}_{\boldsymbol{y}^m \boldsymbol{y}'^n}^{(m+n)} \left(\mathcal{F}(\tau_1), \cdots, \mathcal{F}(\tau_{m+n}) \right).
\end{aligned}$$

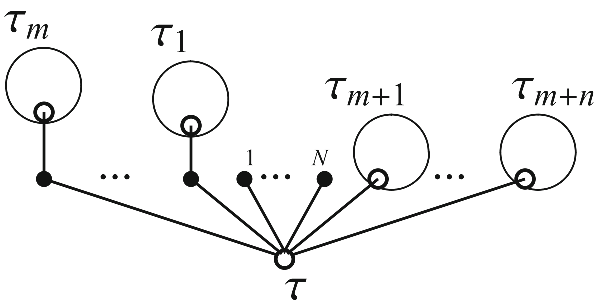


Fig. 2 The mode of the trees with meagre vertices disappearing

Table 6 Tri-coloured Trees which are appended to the set N-T_5 to form the set IEN-T_5

Clearly, the IEN-T set is really an extension of the N-T set (see, Table 14.3 on p.292 in [28]). It can also be seen from Tables 5 and 6 that one 4th-order tree and six 5th-order trees are appended to the N-T set to form the IEN-T set. All these special and new appended trees have a meagre vertex (or some vertices) which correspond to nothing in the N-T set. In fact, the weights Φ_i in Table 6 are all functions of $\bar{a}_{ij}^{(2k)}$ and $a_{ij}^{(2k)}$, the functions of higher-order derivatives of $\bar{a}_{ij}(V)$ and $a_{ij}(V)$ with respect to h.

4.3 The IEN-T set and the EN-T set

First of all, it should be pointed out that there are just five mappings defined on the EN-T set in the paper [25] while six mappings on the IEN-T set in this paper. In the paper [25], the authors introduced *the signed density* $\tilde{\gamma}(\tau)$, but in this paper, we replace $\tilde{\gamma}(\tau)$ by the product of the two mappings, the density $\gamma(\tau)$ and the sign $S(\tau)$.

The IEN-T set is a subset of the EN-T set, once one overlooks the (extended) elementary differential $\mathcal{F}(\tau)$ on them.

4.4 The IEN-T set and the SSEN-T set

From the rules of the IEN-T set and of the SSEN-T set (see [26]), if the function $\boldsymbol{f}$ in the system is independent of $\boldsymbol{y}'$, the IEN-T set is exactly the SSEN-T set.

5 B-series for the general ERKN method

In Section 4, we have presented the IEN-T set and on which six mappings are defined. With all these preliminaries, motivated by the concept of B-series, we will give a totally different approach from the one described in [25] to deriving the theory of order conditions for the general ERKN method.

The main results of the theory of B-series have their origins in the profound paper [29] of Butcher in 1972 and then be introduced by Hairer and Wanner [30] in 1974. In what follows, we present the following two elementary theorems.

Theorem 5.1 *With Definition 4.2, $\boldsymbol{f}(\boldsymbol{y}(t+h), \boldsymbol{y}'(t+h))$ is a B-series*

$$\boldsymbol{f}(\boldsymbol{y}(t+h), \boldsymbol{y}'(t+h)) = \sum_{\tau \in IEN\text{-}T} \frac{h^{\rho(\tau)-1}}{(\rho(\tau)-1)!} \alpha(\tau) \mathcal{F}(\tau)(\boldsymbol{y}, \boldsymbol{y}').$$

Proof First, we expand $\boldsymbol{f}(\boldsymbol{y}(t+h), \boldsymbol{y}'(t+h))$ at point $(\hat{\boldsymbol{y}}, \hat{\boldsymbol{y}}')$, with the denotations (7) and (8).

$$\boldsymbol{f}(\boldsymbol{y}(t+h), \boldsymbol{y}'(t+h)) = \sum_{m\geq 0, n\geq 0} \frac{1}{(m+n)!} \boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m \boldsymbol{y}'^n}\Big|_{(\hat{\boldsymbol{y}},\hat{\boldsymbol{y}}')} \left(\boldsymbol{y}(t+h) - \hat{\boldsymbol{y}}\right)^{\otimes m} \otimes \left(\boldsymbol{y}'(t+h) - \hat{\boldsymbol{y}}'\right)^{\otimes n}, \tag{10}$$

where the second term $\boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m \boldsymbol{y}'^n}\Big|_{(\hat{\boldsymbol{y}},\hat{\boldsymbol{y}}')}$ in this series is the matrix-valued function of h.

Definition 4.2 ensures that $\boldsymbol{f}(\boldsymbol{y}(t+h), \boldsymbol{y}'(t+h))$ is a B-series. In fact, if $\boldsymbol{f}(\boldsymbol{y}(t+h), \boldsymbol{y}'(t+h))$ is a B-series, from the matrix-variation-of-constants formula with $\mu = 1$, (see [25]), and from the properties of the ϕ-functions (see e.g. [2]), we have

$$\begin{aligned}
\boldsymbol{y}(t+h) - \hat{\boldsymbol{y}} &= h^2 \int_0^1 (1-z)\phi_1((1-z)^2 V)\boldsymbol{f}(\boldsymbol{y}(t+hz), \boldsymbol{y}'(t+hz))\mathrm{d}z \\
&= \sum_{\tau\in\text{IEN-T}} \int_0^1 (1-z)\phi_1((1-z)^2 V)\frac{z^{\rho(\tau)-1}}{(\rho(\tau)-1)!}\mathrm{d}z \cdot \left(h^{\rho(\tau)+1}\alpha(\tau)\mathcal{F}(\tau)(\boldsymbol{y}, \boldsymbol{y}')\right) \\
&= \sum_{\tau\in\text{IEN-T}} \phi_{\rho(\tau)+1}(V)\cdot h^{\rho(\tau)+1}\alpha(\tau)\mathcal{F}(\tau)(\boldsymbol{y}, \boldsymbol{y}') \\
&= \sum_{\tau\in\text{IEN-T}} \sum_{p\geq 0} \frac{(-1)^p V^p}{(\rho(\tau)+1+2p)!} h^{\rho(\tau)+1}\alpha(\tau)\mathcal{F}(\tau)(\boldsymbol{y}, \boldsymbol{y}'),
\end{aligned} \tag{11}$$

and

$$\boldsymbol{y}'(t+h) - \hat{\boldsymbol{y}}' = \sum_{\tau\in\text{IEN-T}} \sum_{q\geq 0} \frac{(-1)^q V^q}{(\rho(\tau)+2q)!} h^{\rho(\tau)}\alpha(\tau)\mathcal{F}(\tau)(\boldsymbol{y}, \boldsymbol{y}'). \tag{12}$$

Taking the Taylor series of $\boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m \boldsymbol{y}'^n}\Big|_{(\hat{\boldsymbol{y}},\hat{\boldsymbol{y}}')}$ at $h = 0$, and from (11) and (12), the equation (10) becomes

$$\begin{aligned}
\boldsymbol{f}(\boldsymbol{y}(t+h), \boldsymbol{y}'(t+h)) = \sum_{N,n,m} \sum_{\tau\in\text{IEN-T}} & \frac{h^s}{N!(m+n)!} D_h^N \boldsymbol{f}^{(n+m)}_{\boldsymbol{y}^m \boldsymbol{y}'^n} \\
& \times \Bigg(\frac{(-M)^{p_1}\alpha(\tau_1)\mathcal{F}(\tau_1)(\boldsymbol{y})}{(\rho(\tau_1)+1+2p_1)!}, \ldots, \frac{(-M)^{p_m}\alpha(\tau_m)\mathcal{F}(\tau_m)(\boldsymbol{y})}{(\rho(\tau_m)+1+2p_m)!}, \\
& \frac{(-M)^{q_1}\alpha(\tau_{m+1})\mathcal{F}(\tau_{m+1})(\boldsymbol{y})}{(\rho(\tau_{m+1})+2q_1)!}, \ldots, \frac{(-M)^{q_n}\alpha(\tau_{m+n})\mathcal{F}(\tau_{m+n})(\boldsymbol{y})}{(\rho(\tau_{m+n})+2q_n)!} \Bigg),
\end{aligned} \tag{13}$$

where $s = N + \sum_{k=1}^{m}(2p_k + \rho(\tau_k) + 1) + \sum_{k=1}^{n}(2q_k + \rho(\tau_{m+k}))$. By Definition 4.2, the proof is complete. □

Theorem 5.2 *Given a general ERKN method (5), by Definition 4.2, each* $\boldsymbol{f}(Y_i, Y_i')$ *is a series of the form*

$$\boldsymbol{f}(Y_i, Y_i') = \sum_{\tau\in\textit{IEN-T}} \frac{h^{\rho(\tau)-1}}{\rho(\tau)!}\boldsymbol{a}_i(\tau),$$

where $\boldsymbol{a}_i(\tau) = \Phi_i(\tau) \cdot \gamma(\tau) \cdot S(\tau) \cdot \alpha(\tau) \cdot \mathcal{F}(\tau)(\boldsymbol{y}_n, \boldsymbol{y}'_n)$.

Proof Similarly to the proof of Theorem 5.1, we expand $\boldsymbol{f}(Y_i, Y'_i)$ at $(\tilde{\boldsymbol{y}}, \tilde{\boldsymbol{y}}')$ for the general ERKN method (5), where $\tilde{\boldsymbol{y}} = \phi_0(c_i^2 V)\boldsymbol{y}_n + \phi_1(c_i^2 V)c_i h \boldsymbol{y}'_n$ and $\tilde{\boldsymbol{y}}' = \phi_0(c_i^2 V)\boldsymbol{y}'_n - c_i h M \phi_1(c_i^2 V)\boldsymbol{y}_n$ and obtain the Taylor series expansion as follows:

$$\boldsymbol{f}(Y_i, Y'_i) = \sum_{m,n\geq 0} \frac{1}{(m+n)!} \boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m \boldsymbol{y}'^n}\Big|_{\tilde{\boldsymbol{y}},\tilde{\boldsymbol{y}}'} \left(h^2 \sum_j \bar{a}_{ij}(V)\boldsymbol{f}(Y_j, Y'_j)\right)^{\otimes m} \otimes \left(h \sum_j a_{ij}(V)\boldsymbol{f}(Y_j, Y'_j)\right)^{\otimes n}, \tag{14}$$

where the second term $\boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m \boldsymbol{y}'^n}\Big|_{\tilde{\boldsymbol{y}},\tilde{\boldsymbol{y}}'}$ is the function of $c_i h$. Then, the Taylor series expansion of $\boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m \boldsymbol{y}'^n}\Big|_{(\hat{\boldsymbol{y}},\hat{\boldsymbol{y}}')}$ at $h = 0$ is given by

$$\boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m \boldsymbol{y}'^n}\Big|_{(\hat{\boldsymbol{y}},\hat{\boldsymbol{y}}')} = \sum_{N\geq 0} \frac{c_i^N}{m!} h^N D_h^N \boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m \boldsymbol{y}'^n}. \tag{15}$$

Definition 4.2 ensures that each $\boldsymbol{f}(Y_i, Y'_i)$ for $i = 1, \ldots, s$ is a B-series. In fact, the third and fourth terms in the equation (14) are given by

$$h^2 \sum_j \bar{a}_{ij}(V)\boldsymbol{f}(Y_j, Y'_j) = \sum_{\tau\in\text{IEN-T}} \sum_{p\geq 0} \frac{\sum_j \bar{a}_{ij}^{(2p)}}{\rho(\tau)!} \frac{V^p}{(2p)!} h^{\rho(\tau)+1} \boldsymbol{a}_j(\tau), \tag{16}$$

and

$$h \sum_j a_{ij}(V)\boldsymbol{f}(Y_j, Y'_j) = \sum_{\tau\in\text{IEN-T}} \sum_{q\geq 0} \frac{\sum_j a_{ij}^{(2q)}}{\rho(\tau)!} \frac{V^q}{(2q)!} h^{\rho(\tau)} \boldsymbol{a}_j(\tau). \tag{17}$$

We then obtain

$$\begin{aligned}\boldsymbol{f}(Y_i, Y'_i) = \sum_{N,n,m} \sum_{\tau\in\text{IEN-T}} \frac{c_i^N h^s}{N!(n+m)!} D_h^N \boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m \boldsymbol{y}'^n} \Bigg(& \frac{\sum_j \bar{a}_{ij}^{(2p_1)}}{\rho(\tau_1)!} \frac{M^{p_1}}{(2p_1)!} \boldsymbol{a}_j(\tau_1), \ldots, \frac{\sum_j \bar{a}_{ij}^{(2p_m)}}{\rho(\tau_m)!} \frac{M^{p_m}}{(2p_m)!} \boldsymbol{a}_j(\tau_m), \\ & \frac{\sum_j a_{ij}^{(2q_1)}}{\rho(\tau_{m+1})!} \frac{M^{q_1}}{(2q_1)!} \boldsymbol{a}_j(\tau_{m+1}), \ldots, \frac{\sum_j a_{ij}^{(2q_n)}}{\rho(\tau_{m+n})!} \frac{M^{q_n}}{(2q_n)!} \boldsymbol{a}_j(\tau_{m+n}) \Bigg),\end{aligned} \tag{18}$$

where $s = N + \sum_{k=1}^{m}(2p_k + \rho(\tau_k) + 1) + \sum_{k=1}^{n}(2q_k + \rho(\tau_{m+k}))$. By Definition 4.2, we complete the proof. □

6 The order conditions for the general ERKN method

Theorem 6.1 *The scheme (5) for the general multi-frequency and multidimensional oscillatory second-order initial value problems (1) has order r if and only if the following conditions*

$$\sum_{i=1}^{s} \bar{b}_i(V)S(\tau)\gamma(\tau)\Phi_i(\tau) = \rho(\tau)!\phi_{\rho(\tau)+1}+O(h^{r-\rho(\tau)}), \quad \forall \tau \in IEN\text{-}T_m,\ m \leq r-1, \tag{19}$$

$$\sum_{i=1}^{s} b_i(V)S(\tau)\gamma(\tau)\Phi_i(\tau) = \rho(\tau)!\phi_{\rho(\tau)} + O(h^{r-\rho(\tau)+1}), \quad \forall \tau \in IEN\text{-}T_m,\ m \leq r, \tag{20}$$

are satisfied.

Proof It follows from the matrix-variation-of-constants formula, Theorem 5.1 and Theorem 5.2 that

$$\boldsymbol{y}_{n+1} = \phi_0(V)\boldsymbol{y}_n+h\phi_1(V)\boldsymbol{y}'_n+\sum_{\tau\in\text{IEN-T}} \frac{h^{\rho(\tau)+1}}{\rho(\tau)!}\sum_{i=1}^{s} \bar{b}_i(V)\Phi_i(\tau)S(\tau)\gamma(\tau)\alpha(\tau)\mathcal{F}(\tau)(\boldsymbol{y}_n, \boldsymbol{y}'_n), \tag{21}$$

$$\begin{aligned}\boldsymbol{y}(t+h) \;=\; &\phi_0(V)\boldsymbol{y} + h\phi_1(V)\boldsymbol{y}' + \sum_{\tau\in\text{IEN-T}} h^{\rho(\tau)+1}\alpha(\tau)\mathcal{F}(\tau)(\boldsymbol{y}, \boldsymbol{y})\int_0^1 (1-z)\\ &\times \frac{z^{\rho(\tau)-1}}{(\rho(\tau)-1)!}\phi_1((1-z)V)\,\mathrm{d}z.\end{aligned} \tag{22}$$

Comparing the equations (21) with (22) and using the properties of the ϕ-functions, we obtain the first result of Theorem 6.1. Likewise, we can get the second result of this theorem. □

Theorem 6.1 in this paper and the theorem 4.1 in [25] share the same expression. However, it should be noticed that there exist redundant order conditions in [25]. While any order condition in this paper cannot be replaced by others provided the entries $\bar{a}_{ij}(V)$, $a_{ij}(V)$, $b_i(V)$, and $\bar{b}_i(V)$ in the general ERKN method (5) are independent. Obviously, the disappearing of redundant order conditions can make the construction of high-order general ERKN methods (5) much clearer and simpler.

It is easy to see that Theorem 6.1 implies the order conditions for the standard ERKN methods in [10, 26] once the right-hand side function $\boldsymbol{f}$ does not depend on $\boldsymbol{y}'$. It is noted that, if the matrix M is null, Theorem 6.1 reduces to that for the classical general RKN method when applied to $\boldsymbol{y}'' = \boldsymbol{f}(\boldsymbol{y}, \boldsymbol{y}')$, since the IEN-T set is exactly the N-T set in this special case.

7 The construction of general ERKN methods

In this section, using Theorem 6.1, we present some general ERKN methods (5) of order up to four. The approach to constructing new methods in this section is different from that described in [25].

7.1 Second-order general ERKN methods

From Theorem 6.1 and the three IEN-Ts with order no more than two which are listed in Table 5, for an s-stage general ERKN method (5) expressed in the Butcher tableau (6), we have the second-order conditions as follows:

$$\sum_{i=1}^{s} \bar{b}_i(V) = \phi_2(V) + O(h), \quad \sum_{i=1}^{s} b_i(V) = \phi_1(V) + O(h^2),$$
$$\sum_{i=1}^{s} b_i(V)c_i = \phi_2(V) + O(h), \; \sum_{i=1}^{s} b_i(V)a_{ij}^{(0)} = \phi_2(V) + O(h).$$

Comparing the coefficients of h^0 and h, we obtain four equations:

$$\sum_{i=1}^{s} \bar{b}_i^{(0)} = \frac{1}{2}, \quad \sum_{i=1}^{s} b_i^{(0)} = 1, \quad \sum_{i=1}^{s} b_i^{(0)} c_i = \frac{1}{2}, \quad \sum_{i=1}^{s} b_i^{(0)} a_{ij}^{(0)} = \frac{1}{2}.$$

It can be observed that all these equations are exactly the second-order conditions for the following general RKN method

$$\begin{aligned}
Y_i &= \boldsymbol{y}_n + c_i h \boldsymbol{y}_n' + h^2 \sum_{j=1}^{s} \bar{a}_{ij}^{(0)} \left(\boldsymbol{f}(Y_j, Y_j') - MY_j \right), \qquad i = 1, \cdots, s, \\
Y_i' &= \boldsymbol{y}_n' + h \sum_{j=1}^{s} a_{ij}^{(0)} \left(\boldsymbol{f}(Y_j, Y_j') - MY_j \right), \qquad i = 1, \cdots, s, \\
\boldsymbol{y}_{n+1} &= \boldsymbol{y}_n + h \boldsymbol{y}_n' + h^2 \sum_{i=1}^{s} \bar{b}_i^{(0)} \left(\boldsymbol{f}(Y_i, Y_i') - MY_i \right), \\
\boldsymbol{y}_{n+1}' &= \boldsymbol{y}_n' + h \sum_{i=1}^{s} b_i^{(0)} \left(\boldsymbol{f}(Y_i, Y_i') - MY_i \right),
\end{aligned} \tag{23}$$

when applied to the initial value problems (1), with the Butcher tableau

$$\begin{array}{c|cccc|cccc}
c_1 & \bar{a}_{11}^{(0)} & \bar{a}_{12}^{(0)} & \cdots & \bar{a}_{1s}^{(0)} & a_{11}^{(0)} & a_{12}^{(0)} & \cdots & a_{1s}^{(0)} \\
c_2 & \bar{a}_{21}^{(0)} & \bar{a}_{22}^{(0)} & \cdots & \bar{a}_{2s}^{(0)} & a_{21}^{(0)} & a_{22}^{(0)} & \cdots & a_{2s}^{(0)} \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
c_s & \bar{a}_{s1}^{(0)} & \bar{a}_{s2}^{(0)} & \cdots & \bar{a}_{s,s}^{(0)} & a_{s1}^{(0)} & a_{s2}^{(0)} & \cdots & a_{s,s}^{(0)} \\
\hline
 & \bar{b}_1^{(0)} & \bar{b}_2^{(0)} & \cdots & \bar{b}_s^{(0)} & b_1^{(0)} & b_2^{(0)} & \cdots & b_s^{(0)}
\end{array} . \tag{24}$$

This means that we can easily solve $\left(c_i, \bar{a}_{ij}^{(0)}, a_{ij}^{(0)}, \bar{b}_i^{(0)}, b_i^{(0)}\right)$ in terms of a classical general RKN method. For example, from the explicit 2 stage 2nd-order general RKN method with the Buthcher tableau

$$\begin{array}{c|cc|cc}
0 & & & & \\
\frac{2}{3} & 0 & & \frac{2}{3} & \\
\hline
 & \frac{1}{4} & \frac{3}{4} & \frac{1}{4} & \frac{1}{4}
\end{array} , \tag{25}$$

we can yield the 2 stage 2nd-order explicit general ERKN methods. Two examples are given below.

Example 1 The first 2 stage 2nd-order explicit general ERKN method (5) has its Butcher tableau

$$\begin{array}{c|cc|cc} 0 & & & & \\ \frac{2}{3} & 0 & & \frac{2}{3}I & \\ \hline & \frac{1}{4}I & \frac{3}{4}I & \frac{1}{4}I & \frac{1}{4}I \end{array} . \tag{26}$$

Example 2: The Butcher tableau of the second one is

$$\begin{array}{c|cc|cc} 0 & & & & \\ \frac{2}{3} & 0 & & \frac{2}{3}\phi_0(\frac{4}{9}V) & \\ \hline & \frac{1}{4}\phi_1(V) & \frac{3}{4}\phi_1(\frac{1}{9}V) & \frac{1}{4}\phi_0(V) & \frac{1}{4}\phi_0(\frac{1}{9}V) \end{array} . \tag{27}$$

7.2 Third-order general ERKN methods

From Theorem 6.1 and 9 trees in the set of IEN-T$_m$, $(m \le 3)$ in Table 5, for an s-stage general ERKN method (5) expressed in the Butcher tableau (6), we have the third-order conditions as follows:

$$\sum_{i=1}^{s} \bar{b}_i(V) = \phi_2(V) + O(h^2), \qquad \sum_{i=1}^{s} \bar{b}_i(V)c_i = \phi_3(V) + O(h),$$
$$\sum_{i=1}^{s}\sum_{j=1}^{s} \bar{b}_i(V)a_{ij}^{(0)} = \phi_3(V) + O(h),$$
$$\sum_{i=1}^{s} b_i(V) = \phi_1(V) + O(h^3), \qquad \sum_{i=1}^{s} b_i(V)c_i = \phi_2(V) + O(h^2),$$
$$\sum_{i=1}^{s}\sum_{j=1}^{s} b_i(V)a_{ij}^{(0)} = \phi_2(V) + O(h^2),$$
$$\sum_{i=1}^{s} b_i(V)c_i^2 = 2\phi_3(V) + O(h), \qquad \sum_{i=1}^{s}\sum_{j=1}^{s} b_i(V)c_i a_{ij}^{(0)} = 2\phi_3(V) + O(h),$$
$$\sum_{i=1}^{s}\sum_{j=1}^{s}\sum_{k=1}^{s} b_i(V)a_{ij}^{(0)}a_{ik}^{(0)} = 2\phi_3(V) + O(h),$$
$$\sum_{i=1}^{s} b_i(V)\bar{a}_{ij}^{(0)} = \phi_3(V) + O(h), \qquad \sum_{i=1}^{s}\sum_{j=1}^{s} b_i(V)a_{ij}^{(0)}c_j = \phi_3(V) + O(h),$$
$$\sum_{i=1}^{s}\sum_{j=1}^{s}\sum_{k=1}^{s} b_i(V)a_{ij}^{(0)}a_{jk}^{(0)} = \phi_3(V) + O(h).$$

Comparing the coefficients of the power of h, we obtain 13 equations, where 12 equations are exactly the third-order conditions for the classical general RKN method (23) with the Butcher tableau (24)

$$\sum_{i=1}^{s} \bar{b}_i^{(0)} \gamma(\tau)\Phi_i(\tau) = \frac{1}{\rho(\tau)+1}, \quad \forall \tau \in \text{N-T}_m,\ m \le 2, \tag{28}$$

$$\sum_{i=1}^{s} b_i^{(0)} \gamma(\tau)\Phi_i(\tau) = 1, \quad \forall \tau \in \text{N-T}_m,\ m \le 3, \tag{29}$$

together with the last equation $\sum_{i=1}^{s} \bar{b}_i^{(2)} = -\frac{1}{3}$. We can solve $\left(c_i, \bar{a}_{ij}^{(0)}, a_{ij}^{(0)}, \bar{b}_i^{(0)}, b_i^{(0)}\right)$ from the equations (28) and (29) via a classical general RKN method. We then can solve $b_i^{(2)}$ from the last equation. In such kind of approach, we complete the construction of the general ERKN methods of order three. For example, from the explicit 3 stage 3rd-order general RKN method with the Buthcher tableau

$$\begin{array}{c|ccc|ccc} 0 & & & & & & \\ \frac{1}{2} & 0 & & & \frac{1}{2} & & \\ 1 & 1 & 0 & & -1 & 2 & \\ \hline & \frac{1}{6} & \frac{2}{6} & 0 & \frac{1}{6} & \frac{4}{6} & \frac{1}{6} \end{array} \tag{30}$$

we can construct the 3 stage 3rd-order explicit general ERKN methods straightforwardly. The three examples are listed below.

Example 3 The first 3 stage 3rd-order explicit general ERKN method (5) is expressed in the Butcher tableau

$$\begin{array}{c|ccc|ccc} 0 & & & & & & \\ \frac{1}{2} & 0 & & & \frac{1}{2}I & & \\ 1 & I & 0 & & -I & 2I & \\ \hline & \frac{1}{6}I & \frac{2}{6}I & 0 & \frac{1}{6}(I-\frac{9}{20}V) & \frac{4}{6}(I-\frac{3}{20}V) & \frac{1}{6}(I+\frac{1}{20}V) \end{array}. \tag{31}$$

Example 4 The Butcher tableau of the second 3 stage 3rd-order explicit general ERKN method (5) is given by

$$\begin{array}{c|ccc|ccc} 0 & & & & & & \\ \frac{1}{2} & 0 & & & \frac{1}{2}I & & \\ 1 & I & 0 & & -I & 2I & \\ \hline & \frac{1}{6}(I-\frac{1}{6}V) & \frac{2}{6}(I-\frac{1}{24}V) & 0 & \frac{1}{6}(I-\frac{1}{2}V) & \frac{4}{6}(I-\frac{1}{8}V) & \frac{1}{6}I \end{array}. \tag{32}$$

Example 5 The third 3 stage 3rd-order explicit general ERKN method (5) is denoted by the Butcher tableau

$$\begin{array}{c|ccc|ccc} 0 & & & & & & \\ \frac{1}{2} & 0 & & & \frac{1}{2}\phi_0(\frac{1}{4}V) & & \\ 1 & \phi_1(V) & 0 & & -\phi_0(V) & 2\phi_0(\frac{1}{4}V) & \\ \hline & \frac{1}{6}\phi_1(V) & \frac{2}{6}\phi_1(\frac{1}{4}V) & 0 & \frac{1}{6}\phi_0(V) & \frac{4}{6}\phi_0(\frac{1}{4}V) & \frac{1}{6}I \end{array}. \tag{33}$$

7.3 Fourth-order general ERKN methods

From Theorem 6.1 and Table 5, comparing the coefficients of the power of h of (19) and (20), for an s-stage general ERKN method (5) with the coefficient $\left(\bar{a}_{ij}(V), a_{ij}(V), \bar{b}_i(V), b_i(V)\right)$ displayed in the Butcher tableau (6), we can obtain 41 fourth-order conditions, in which 36 conditions are listed as follows:

$$\sum_{i=1}^{s} \bar{b}_i^{(0)} \gamma(\tau)\Phi_i(\tau) = \frac{1}{\rho(\tau)+1}, \quad \forall \tau \in \text{N-T}_m,\ m \leq 3, \tag{34}$$

$$\sum_{i=1}^{s} b_i^{(0)} \gamma(\tau)\Phi_i(\tau) = 1, \quad \forall \tau \in \text{N-T}_m,\ m \leq 4, \tag{35}$$

and the other five conditions are given below

$$\begin{aligned} &\sum_{i=1}^{s}\sum_{j=1}^{s} b_i^{(0)} a_{ij}^{(2)} = -\frac{1}{12},\ \sum_{i=1}^{s} b_i^{(2)} = -\frac{1}{3},\ \sum_{i=1}^{s} b_i^{(2)} c_i = -\frac{1}{12},\\ &\sum_{i=1}^{s}\sum_{j=1}^{s} b_i^{(2)} a_{ij}^{(0)} = -\frac{1}{12},\ \sum_{i=1}^{s} \bar{b}_i^{(2)} = -\frac{1}{12}. \end{aligned} \tag{36}$$

For each specific classical general RKN method of order 4, we can solve $\left(c_i, \bar{a}_{ij}^{(0)}, a_{ij}^{(0)}, \bar{b}_i^{(0)}, b_i^{(0)}\right)$ from (34) and (35), since these 36 conditions are exactly the order conditions for the classical general RKN method (23) with the Butcher tableau (24). Then, we can solve $\left(a_{ij}^{(2)}, \bar{b}_i^{(2)}, b_i^{(2)}\right)$ from conditions (36). In this way, we construct the general ERKN methods (5) of order 4.

In what follows, we will gain explicit 4 stage 4th-order general ERKN methods from the following explicit 4 stage 4th-order classical general RKN method (23) with the Butcher tableau

$$\begin{array}{c|cccc|cccc} 0 & & & & & & & & \\ \frac{1}{2} & \frac{1}{8} & & & & \frac{1}{2} & & & \\ \frac{1}{2} & \frac{1}{8} & 0 & & & 0 & \frac{1}{2} & & \\ 1 & 0 & 0 & \frac{1}{2} & & 0 & 0 & 1 & \\ \hline & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & 0 & \frac{1}{6} & \frac{2}{6} & \frac{2}{6} & \frac{1}{6} \end{array}\ . \tag{37}$$

Some general ERKN methods of order four constructed in this approach are shown below.

Example 6 The Butcher tableau of the first explicit 4 stage 4th-order general ERKN method (5) is given by

$$\begin{array}{c|cccc|cccc} 0 & & & & & & & & \\ \frac{1}{2} & \frac{1}{8}I & & & & \frac{1}{2}I & & & \\ \frac{1}{2} & \frac{1}{8}I & 0 & & & 0 & \frac{1}{2}I & & \\ 1 & 0 & 0 & \frac{1}{2}I & & 0 & 0 & I-\frac{1}{4}V & \\ \hline & \frac{1}{6}(I-\frac{1}{12}V) & \frac{1}{6}(I-\frac{1}{12}V) & \frac{1}{6}(I-\frac{1}{12}V) & 0 & \frac{1}{6}(I-\frac{1}{2}V) & \frac{2}{6}(I-\frac{1}{8}V) & \frac{2}{6}(I-\frac{1}{8}V) & \frac{1}{6}I \end{array}\ . \tag{38}$$

Example 7 The second explicit 4 stage 4th-order general ERKN method is expressed in the Butcher tableau

$$
\begin{array}{c|cccc|cccc}
0 & & & & & & & & \\
\frac{1}{2} & \frac{1}{8}I & & & & \frac{1}{2}(I-\frac{1}{8}V) & & & \\
\frac{1}{2} & \frac{1}{8}I & 0 & & & 0 & \frac{1}{2}I & & \\
1 & 0 & 0 & \frac{1}{2}I & & 0 & 0 & I-\frac{1}{8}V & \\
\hline
 & \frac{1}{6}(I-\frac{1}{6}V) & \frac{1}{6}(I-\frac{1}{24}V) & \frac{1}{6}(I-\frac{1}{24}V) & 0 & \frac{1}{6}(I-\frac{1}{2}V) & \frac{2}{6}(I-\frac{1}{8}V) & \frac{2}{6}(I-\frac{1}{8}V) & \frac{1}{6}I
\end{array}
\quad . \tag{39}
$$

Example 8 The third explicit 4 stage 4th-order general ERKN method (5) has the Butcher tableau as follows:

$$
\begin{array}{c|cccc|cccc}
0 & & & & & & & & \\
\frac{1}{2} & \frac{1}{8}\phi_1(\frac{1}{4}V) & & & & \frac{1}{2}\phi_0(\frac{1}{4}V) & & & \\
\frac{1}{2} & \frac{1}{8}\phi_1(\frac{1}{4}V) & 0 & & & 0 & \frac{1}{2}I & & \\
1 & 0 & 0 & \frac{1}{2}\phi_1(\frac{1}{4}V) & & 0 & 0 & \phi_0(\frac{1}{4}V) & \\
\hline
 & \frac{1}{6}\phi_1(V) & \frac{1}{6}\phi_1(\frac{1}{4}V) & \frac{1}{6}\phi_1(\frac{1}{4}V) & 0 & \frac{1}{6}\phi_0(V) & \frac{2}{6}\phi_0(\frac{1}{4}V) & \frac{2}{6}\phi_0(\frac{1}{4}V) & \frac{1}{6}I
\end{array}
\quad . \tag{40}
$$

7.4 An effective approach to constructing the general ERKN methods

In the paper [25], in order to construct fourth-order general ERKN methods for the systems (1), the authors first considered all 62 graphs of the EN-Ts (see Tables 1 and 2 in [25]), and then selected and deleted 34 redundant trees. Finally, they obtained 28 non-redundant EN-Ts (see Tables 3 and 4 in [25]). With these 28 EN-Ts, the authors in [25] achieved special fourth-order conditions, and then the authors derived an fourth-order ERKN method under two auxiliary simplifying assumptions.

Obviously, as shown in paper [25], more than half of the time and effort spent on drawing the redundant trees. In a word, the process described in paper [25] is difficult to follow since the number of the redundant trees in the EN-T set is much huge.

However, in this paper, these 28 trees can be directly obtained since 27 of them are exactly the classical N-Ts as shown in Section 4.2. In this way, it becomes quite easy to get the fourth-order conditions for the general ERKN method (5). Then using the expansions of these order conditions with respect to the power of h, we can check that some are exactly the order conditions for the classical general RKN method (23). This approach to constructing the general ERKN integrators is very effective and efficient in practice as shown in the previous subsections where second-, third- and fourth-order general ERKN methods are constructed as examples.

8 Numerical experiments

In this section, some numerical experiments are implemented to illustrate that the general ERKN methods (5) are competitive in comparison with the others in the literature. The criterion used in the numerical comparisons is the base-10 logarithm of the maximum global error ($\log_{10} \|\mathrm{MGE}\|$) versus the base-2 logarithm of the stepsizes ($\log_2(h)$). The following 11 methods are used to solve the general system (1) for the comparison:

- RKN2: The 2 stage 2nd-order general RKN method (25).
- ERKN2a: The first 2 stage 2nd-order general ERKN method (26) given in Section 7 of this paper.
- ERKN2b: The second 2 stage 2nd-order general ERKN method (27) given in Section 7 of this paper.
- RKN3: The 3 stage 3rd-order general RKN method (30).
- ERKN3a: The first 3 stage 3rd-order general ERKN method (31) given in Section 7 of this paper.
- ERKN3b: The second 3 stage 3rd-order general ERKN method (32) given in Section 7 of this paper.
- ERKN3c: The third 3 stage 3rd-order general ERKN method (33) given in Section 7 of this paper.
- RKN4: The 4 stage 4th-order general RKN method (37).
- ERKN4a: The first 4 stage 4th-order general ERKN method (38) given in Section 7 of this paper.
- ERKN4b: The second 4 stage 4th-order general ERKN method (39) given in Section 7 of this paper.
- ERKN4c: The third 4 stage 4th-order general ERKN method (40) given in Section 7 of this paper.

Problem 1 We consider the damped equation

$$my'' + by' + ky = 0,$$

as one of the test problems. When the damping constant b is small, we would expect the system to still oscillate, but with decreasing amplitude as its energy is converted to heat. In this numerical test, the problem is integrated on the interval $[0, 300]$ with $m = 1$, $b = 0.01$, $k = 3$ and the initial conditions $\big(y(0), y'(0)\big) = (1, 0)$. The analytic solution to the problem is given by

$$y(t) = e^{-\frac{0.01}{2}t}\left(\cos\left(\frac{\sqrt{12-0.01^2}}{2}t\right) + \frac{0.01}{\sqrt{12-0.01^2}}\sin\left(\frac{\sqrt{12-0.01^2}}{2}t\right)\right).$$

The numerical results are displayed in Fig. 3, where the small stepsizes for the methods are $h = \frac{1}{2^j}$ for $j = 3, \ldots, 8$ and the big stepsizes are $h = \frac{j}{8}$ for $j = 2, \ldots, 6$.

Problem 2 We consider the initial value problem

$$y''(t)+\begin{pmatrix} 13 & -12 \\ -12 & 13 \end{pmatrix} y(t) = \frac{12\varepsilon}{5}\begin{pmatrix} 3 & 2 \\ -2 & -3 \end{pmatrix} y'(t)+\varepsilon^2\begin{pmatrix} \frac{36}{5}\sin(t) + 24\sin(5t) \\ -\frac{24}{5}\sin(t) - 36\sin(5t) \end{pmatrix},$$

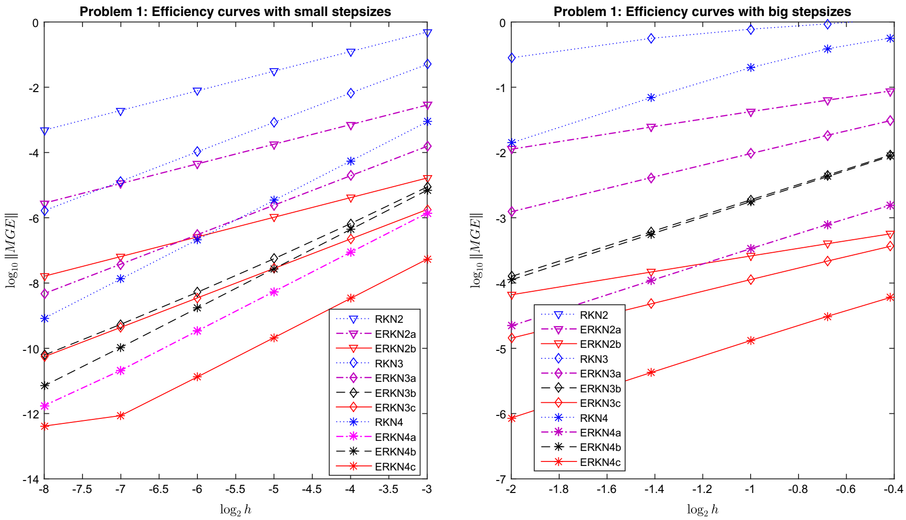


Fig. 3 Problem 1 integrated on [0, 300]

with the initial values $y(0) = (\varepsilon, \varepsilon)^\intercal$ and $y'(0) = (-4, 6)^\intercal$. The analytic solution is given by

$$y(t) = \begin{pmatrix} \sin(t) - \sin(5t) + \varepsilon \cos(t) \\ \sin(t) + \sin(5t) + \varepsilon \cos(5t) \end{pmatrix}.$$

In the numerical experiment, we choose the parameter value $\varepsilon = 10^{-3}$ and integrate this problem on the interval [0, 300]. The numerical results are displayed in Fig. 4. The small stepsizes are $h = \frac{1}{2^j}$ for $j = 3, \ldots, 8$ and the big stepsizes are $h = \frac{j}{8}$ for

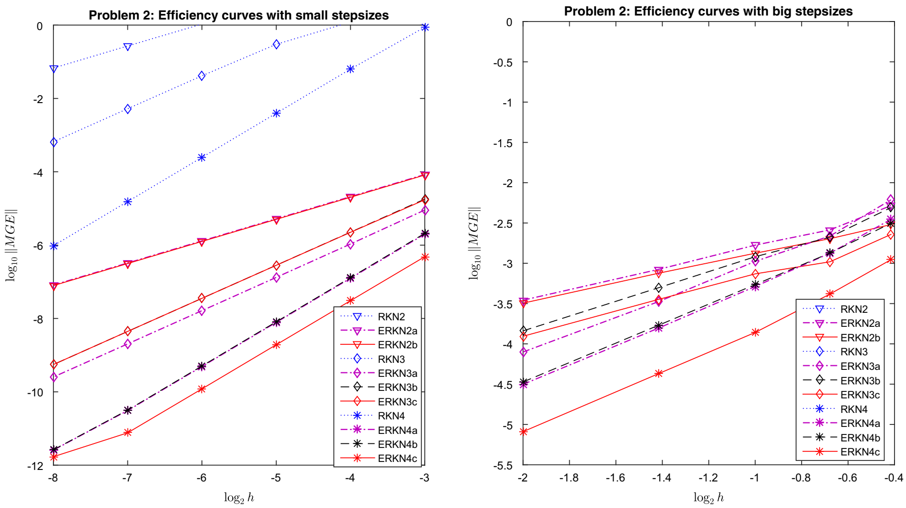


Fig. 4 Problem 2 integrated on [0, 300]

$j = 2, \ldots, 6$. In this numerical test with the big stepsizes, the classical general RKN methods (RKN2, RKN3 and RKN4) give disappointed numerical results. Thus, we do not depict the corresponding points in Fig. 4.

Problem 3 Consider the damped wave equation with periodic conditions (wave propagation in a medium, see e.g. Weinberger [31])

$$\begin{cases} \dfrac{\partial^2 u}{\partial t^2} + \delta \dfrac{\partial u}{\partial t} = \dfrac{\partial^2 u}{\partial x^2} - f(u), \quad -1 < x < 1, \ t > 0, \\ u(-1, t) = u(1, t), \end{cases}$$

where $f(u) = -\sin u$,the damped sine Gordon equation, and $\delta = 1$. A semi-discretization in the spatial variable by second-order symmetric differences leads to the following system of second-order ODEs in time

$$\ddot{U} + MU = F(U, \dot{U}), \quad 0 < t \leq t_{end},$$

where $U(t) = (u_1(t), \cdots, u_N(t))^{\mathsf{T}}$ with $u_i(t) \approx u(x_i, t), \ i = 1, \ldots, N$,

$$M = \frac{1}{\triangle x^2} \begin{pmatrix} 2 & -1 & & & -1 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ -1 & & & -1 & 2 \end{pmatrix},$$

$\triangle x = 2/N$, $x_i = -1 + i\triangle x$ and $F(U, \dot{U}) = (f(u_1) - \delta \dot{u}_1, \cdots, f(u_N) - \delta \dot{u}_N)^{\mathsf{T}}$. Following the paper [32], we take the initial conditions as

$$U(0) = (\pi, \cdots, \pi)^{\mathsf{T}}, \quad U_t(0) = \sqrt{N}\left(0.01 + \sin\left(\frac{2\pi}{N}\right), \cdots, 0.01 + \sin\left(\frac{2\pi N}{N}\right)\right)^{\mathsf{T}},$$

with $N = 64$ and integrate the problem on the interval $[0, 300]$ with small stepsizes $h = \frac{1}{2^j}$ for $j = 5, \ldots, 8$ and with big stepsizes $h = \frac{j}{128}$ for $j = 5, 6, 8, 10$. The numerical results are displayed in Fig. 5. In this numerical test for the big stepsizes, the classical general RKN methods (RKN2, RKN3 and RKN4) all behave badly, with enormous errors.

It can be observed from Figs. 3, 4 and 5 that

- The general ERKN methods perform more efficiently than the classical general RKN methods.
- The higher order general ERKN methods are more efficient than the lower ones.
- As the stepsize decreases, the difference among the general ERKN methods of the same order becomes negligible.
- The general ERKN methods behave perfectly for the large stepsizes.

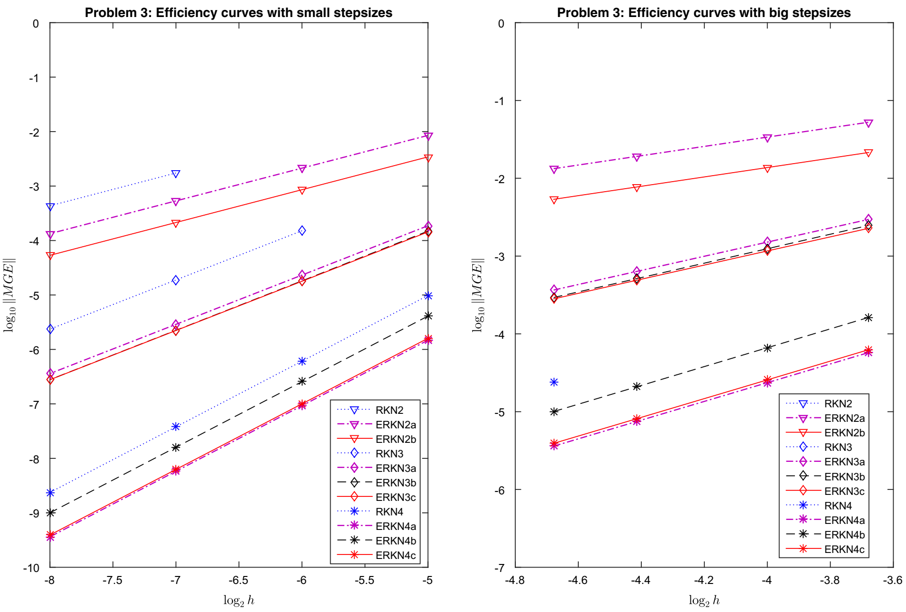


Fig. 5 Problem 3 integrated on [0, 300]

9 Conclusions and discussions

As stated above, in this paper, we have established an improved theory for the order conditions for the general ERKN methods designed specially for solving multi-frequency oscillatory system (1). The original tri-coloured tree theory and the order conditions for the general ERKN methods presented in the paper [25] are not satisfied yet due to the existence of enormous number of redundant trees. This paper has succeeded in the simplification by defining the IEN-T set and on which some special mappings (especially the extended elementary differential mapping) are introduced.

This simplification of the order conditions for the general ERKN methods when applied to the oscillatory system (1) is of great importance. The new tri-coloured tree theory and the B-series theory for the general ERKN methods solving the general system (1) reduce to those for standard ERKN methods solving special system (2), where the right-hand side vector-valued function $\boldsymbol{f}$ does not depend on $\boldsymbol{y}'$ (see [10, 26]).

This successful simplification makes the construction of the general ERKN methods much simpler and more efficient for the system (1). In light of the reduced tree theory analysed in this paper, almost one half of algebraic conditions in the paper [25] can be reduced. Furthermore, in this paper, from the relation between the theories of order conditions for the general RKN method and for the general ERKN method, we propose a simple approach to constructing the new integrators. The numerical results show that the general ERKN methods are more suitable for long-term integration with a large stepsize in comparison with the RKN methods in the literature.

Acknowledgments The authors are grateful to the anonymous referees for their careful reading of the manuscript and for their invaluable comments and suggestions which improved this paper greatly.

The research was supported in part by the Science Foundations of the Nanjing Institute of Technology under Grant CKJA201410 and under Grant QKJA201404, by the Natural Science Foundation of China under Grant 11671200 and 11271186, by NSFC and RS International Exchanges Project under Grant 11411130115, by the Specialized Research Foundation for the Doctoral Program of Higher Education under Grant 20130091110041 and by the 985 Project at Nanjing University under Grant 9112020301.

References

1. Hairer, E., Lubich, C., Wanner, G.: Geometric Numerical Integration. 2nd edn. Springer, Berlin (2006)
2. Wu, X., You, X., Wang, B.: Structure-preserving algorithms for oscillatory differential equations. Springer, Berlin (2013)
3. Wu, X., Liu, K., Shi, W.: Structure-preserving algorithms for oscillatory differential equations II. Springer, Berlin (2015)
4. Shi, W., Wu, X., Xia, J.: Explicit multi-symplectic extended leap-frog methods for Hamiltonian wave equations. J. Comput. Phys. **231**, 7671–7694 (2012)
5. Wu, X., Wang, B., Shi, W.: Effective integrators for nonlinear second-order oscillatory systems with a time-dependent frequency matrix. Appl. Math. Model. **37**, 6505–6518 (2013)
6. Wu, X., Wang, B., Liu, K., Zhao, H.: ERKN methods for long-term integration of multidimensional orbital problems. Appl. Math. Model. **37**, 2327–2336 (2013)
7. Liu, C., Wu, X., An energy-preserving and symmetric scheme for nonlinear Hamiltonian wave equations: J. Math. Anal. Appl. **440**, 167–182 (2016)
8. Wu, X., Liu, C., Mei, L.: A new framework for solving partial differential equations using semi-analytical explicit RK(N)-type integrators. J. Comput. Appl. Math. **301**, 74–90 (2016)
9. Yang, H., Wu, X., You, X., Fang, Y.: Extended RKN-type methods for numerical integration of perturbed oscillators. Comput. Phys. Commun. **180**, 1777–1794 (2009)
10. Wu, X., You, X., Shi, W., Wang, B.: ERKN integrators for systems of oscillatory second-order differential equations. Comput. Phys. Commun. **181**, 1873–1887 (2010)
11. Li, J., Wang, B., You, X., Wu, X.: Two-step extended RKN methods for oscillatory systems. Comput. Phys. Commun. **182**, 2486–2507 (2011)
12. Li, J., Wu, X.: Error analysis of explicit TSERKN methods for highly oscillatory systems. Numer. Algorithms **65**, 465–483 (2014)
13. Li, J., Wu, X.: Adapted Falkner-type methods solving oscillatory second-order differential equations. Numer. Algorithms **62**, 355–381 (2013)
14. Wang, B., Wu, X., Zhao, H.: Novel improved multidimensional Strömer-Verlet formulas with applications to four aspects in scientific computation. Math. Comput. Model. **57**, 857–872 (2013)
15. Wang, B., Wu, X.: A new high precision energy-preserving integrator for system of oscillatory second-order differential equations. Phys. Lett. A. **376**, 1185–1190 (2012)
16. Wu, X., Wang, B., Shi, W.: Efficient energy-preserving integrators for oscillatory Hamiltonian systems. J. Comput. Phys. **235**, 587–605 (2013)
17. Wu, X., Wang, B., Xia, J.: Extended symplectic Runge-Kutta-Nyström integrators for separable Hamiltonian systems. In: Proceedings of the 2010 International Conference on Computational and Mathematical Methods in Science and Engineering, Vol. III, pp. 1016–1020. Spain (2010)
18. Wu, X., Wang, B., Xia, J.: Explicit symplectic multidimensional exponential fitting modified Runge-Kutta-Nyström methods. BIT Numer. Math. **52**, 773–795 (2012)
19. Wang, B., Wu, X.: A highly accurate explicit symplectic ERKN method for multi-frequency and multidimensional oscillatory Hamiltonian systems. Numer. Algorithms **65**, 705–721 (2014)
20. Yang, H., Wu, X.: Trigonometrically-fitted ARKN methods for perturbed oscillators. Appl. Numer. Math. **58**, 1375–1395 (2008)
21. Wu, X., You, X., Xia, J.: Order conditions for ARKN methods solving oscillatory system. Comput. Phys. Commun. **180**, 2250–2257 (2009)
22. Wu, X.: A note on stability of multidimensional adapted Runge-Kutta-Nyström methods for oscillatory systems. Appl. Math. Model. **36**, 6331–6337 (2012)

23. Shi, W., Wu, X.: A note on symplectic and symmetric ARKN methods. Comput. Phys. Comm. **184**, 2408–2411 (2013)
24. Liu, K., Wu, X.: Multidimensional ARKN methods for general oscillatory second-order initial value problems. Comput. Phys. Comm. **185**, 1999–2007 (2014)
25. You, X., Zhao, J., Yang, H., Fang, Y., Wu, X.: Order conditions for RKN methods solving general second-order oscillatory systems. Numer. Algorithms **66**, 147–176 (2014)
26. Yang, H., Zeng, X., Wu, X., Ru, Z.: A simplified Nyström-tree theory for extended Runge-Kutta-Nyström integrators solving multi-frequency oscillatory systems. Comput. Phys. Commun. **185**, 2841–2850 (2014)
27. Boik, R.J.: Lecture notes: statistics 550 spring 2006, http://www.math.montana.edu/~rjboik/classes/550/notes.550.06.pdf, 33–35
28. Hairer, E., Nørsett, S.P., Wanner, G.: Solving ordinary differential equations I, nonstiff problems, end edn., Springer series in Computational Mathematics. Springer, Berlin (1993)
29. Butcher, J.C.: An algebraic theory of integration methods. Math. Comput. **26**, 79–106 (1972)
30. Hairer, E., Wanner, G.: On the Butcher group and general multi-value methods. Computing **13**, 1–15 (1974)
31. Weinberger, H.F.: A First Course in Partial Differential Equations with Complex Variables and Transform Methods. Dover Publications Inc., New York (1965)
32. Franco, J.M.: New methods for oscillatory systems based on ARKN methods. Appl. Numer. Math. **56**, 1040–1053 (2006)