Chapter 8
A Compact Tri-Colored Tree Theory for General ERKN Methods

This chapter develops a compact tri-colored rooted-tree theory for the order conditions for general ERKN methods. The bottleneck of the original tri-colored rooted-tree theory is the existence of numerous redundant trees. This chapter first introduces the extended elementary differential mappings. Then, the new compact tri-colored rooted tree theory is established based on a subset of the original tri-colored rooted-tree set. This new theory makes all redundant trees no longer appear, and hence the order conditions of ERKN methods for general multi-frequency and multidimensional second-order oscillatory systems are greatly simplified.

8.1 Introduction

Runge–Kutta–Nyström (RKN) methods (see [12]) are very popular for solving second-order differential equations. This chapter develops the rooted-tree theory and B-series for *extended Runge–Kutta–Nyström* (ERKN) methods solving general multi-frequency and multi-dimensional oscillatory second-order initial value problems (IVPs) of the form

$$\begin{cases} \boldsymbol{y}''(t) + M\boldsymbol{y}(t) = \boldsymbol{f}\big(\boldsymbol{y}(t), \boldsymbol{y}'(t)\big), & t \in [t_0, T], \\ \boldsymbol{y}(t_0) = \boldsymbol{y}_0, \quad \boldsymbol{y}'(t_0) = \boldsymbol{y}'_0, \end{cases} \tag{8.1}$$

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 position $\boldsymbol{y}$ and velocity $\boldsymbol{y}'$ as arguments. In the special case where the right-hand side function of (8.1) does not depend on velocity $\boldsymbol{y}'$, (8.1) reduces to the following special second-order oscillatory system

X. Wu and B. Wang, *Recent Developments in Structure-Preserving Algorithms for Oscillatory Differential Equations*, https://doi.org/10.1007/978-981-10-9004-2_8

$$\begin{cases} \boldsymbol{y}''(t) + M\boldsymbol{y}(t) = \boldsymbol{f}\big(\boldsymbol{y}(t)\big), & t \in [t_0, T], \\ \boldsymbol{y}(t_0) = \boldsymbol{y}_0, \quad \boldsymbol{y}'(t_0) = \boldsymbol{y}'_0. \end{cases} \tag{8.2}$$

Furthermore, if M is symmetric and positive semi-definite and $\boldsymbol{f}(\boldsymbol{q}) = -\nabla \boldsymbol{U}(\boldsymbol{q})$, then, with $\boldsymbol{q} = \boldsymbol{y}$, $\boldsymbol{p} = \boldsymbol{y}'$, (8.2) becomes identical to a multi-frequency and multidimensional oscillatory Hamiltonian system

$$\begin{cases} \boldsymbol{p}'(t) = -\nabla_{\boldsymbol{q}} H(\boldsymbol{p}(t), \boldsymbol{q}(t)), & \boldsymbol{p}(t_0) = \boldsymbol{p}_0, \\ \boldsymbol{q}'(t) = \quad \nabla_{\boldsymbol{p}} H(\boldsymbol{p}(t), \boldsymbol{q}(t)), & \boldsymbol{q}(t_0) = \boldsymbol{q}_0, \end{cases} \tag{8.3}$$

with the Hamiltonian

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

where $\boldsymbol{U}(\boldsymbol{q})$ is a smooth potential function. For solving the multi-frequency, multidimensional, oscillatory system (8.3), a large number of studies have been made (see, e.g. [6, 25, 28]). The methods for problems (8.1) and (8.2) 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. [11, 14, 26, 27, 29]). 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 the papers [23, 32] to solve the special oscillatory system (8.2). ERKN methods work well 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. [8, 9]), to Falkner-type methods (see, e.g. [7]), to Störmer–Verlet methods (see, e.g. [17]), to energy-preserving methods (see, e.g. [11, 15, 24]), and to symplectic and multi-symplectic methods (see, e.g. [14, 16, 19, 20]). Meanwhile, further research on ARKN methods, including the symplectic conditions and symmetry, has been carried out in the following papers [10, 13, 21, 22, 31].

In a recent paper [33], ERKN methods were extended to the general oscillatory system (8.1), and a tri-colored tree theory called *extended Nyström tree theory* (EN-T theory) was analysed for the order conditions. Unfortunately, however, the EN-T theory is not completely satisfactory due to the existence of redundant trees. For example, there are 7 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 needs to draw all the trees of order up to r first, and then from them select and delete about half of the redundant trees. This will lead to inefficiency in the use of the EN-T theory to achieve the order conditions for ERKN methods.

Hence, in this chapter, we will present an improved theory to eliminate all such redundant trees. In a similar approach to the case of the special oscillatory system

(8.2) in [30], *extended elementary differentials* are required, and we will discuss this in detail in Sect. 8.4.

This chapter is organized as follows. We first summarise the ERKN method for the general oscillatory system (8.1) in Sect. 8.2, and then in Sect. 8.3 we illustrate drawbacks of the EN-T theory proposed in [33]. In Sect. 8.4, we introduce *the set of improved extended-Nyström trees* and show how this relates to other tree sets in the literature. Section 8.5 focuses on the B-series associated with the ERKN method for the general oscillatory system (8.1), and Sect. 8.6 analyses the corresponding order conditions for the ERKN methods, when applied to the general oscillatory system (8.1). In Sect. 8.7 we derive some ERKN methods of order up to four, exploiting the advantages of the new tree theory. The numerical experiments are made in Sect. 8.8. Conclusive remarks are included in Sect. 8.9.

8.2 General ERKN Methods

To begin with, we summarise the following general ERKN method based on the matrix-variation-of-constants formula (see [23]) and quadrature formulae.

Definition 8.1 (*See* [33]) An s-stage general extended Runge–Kutta–Nyström (ERKN) method for the numerical integration of the IVP (8.1) is defined by the following scheme

$$\begin{cases} Y_i = \phi_0(c_i^2 V)\boldsymbol{y}_n + c_i\phi_1(c_i^2 V)h\boldsymbol{y}_n' + h^2\sum_{j=1}^{s}\bar{a}_{ij}(V)\boldsymbol{f}(Y_j, Y_j'), \qquad i = 1,\ldots,s, \\ hY_i' = -c_i V\phi_1(c_i^2 V)\boldsymbol{y}_n + \phi_0(c_i^2 V)h\boldsymbol{y}_n' + h^2\sum_{j=1}^{s}a_{ij}(V)\boldsymbol{f}(Y_j, Y_j'), \qquad i = 1,\ldots,s, \\ \boldsymbol{y}_{n+1} = \phi_0(V)\boldsymbol{y}_n + \phi_1(V)h\boldsymbol{y}_n' + h^2\sum_{i=1}^{s}\bar{b}_i(V)\boldsymbol{f}(Y_i, Y_i'), \\ h\boldsymbol{y}_{n+1}' = -V\phi_1(V)\boldsymbol{y}_n + \phi_0(V)h\boldsymbol{y}_n' + h^2\sum_{i=1}^{s}b_i(V)\boldsymbol{f}(Y_i, Y_i'), \end{cases} \tag{8.4}$$

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 $k = 0, 1, 2, \ldots$.

The ERKN method (8.4) in Definitions 8.1 can also be represented compactly in a Butcher tableau of the coefficients [4]:

$$\begin{array}{c|cccc|cccc} c_1 & \bar{a}_{11}(V) & \bar{a}_{12}(V) & \cdots & \bar{a}_{1s}(V) & a_{11}(V) & a_{12}(V) & \cdots & a_{1s}(V) \\ c_2 & \bar{a}_{21}(V) & \bar{a}_{22}(V) & \cdots & \bar{a}_{2s}(V) & a_{21}(V) & a_{22}(V) & \cdots & a_{2s}(V) \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & \bar{a}_{s1}(V) & \bar{a}_{s2}(V) & \cdots & \bar{a}_{ss}(V) & a_{s1}(V) & a_{s2}(V) & \cdots & a_{ss}(V) \\ \hline & \bar{b}_1(V) & \bar{b}_2(V) & \cdots & \bar{b}_s(V) & b_1(V) & b_2(V) & \cdots & b_s(V) \end{array} \quad . \tag{8.5}$$

In essence, ERKN methods incorporate the particular structure of the oscillatory system (8.1) into both the internal stages and the updates. Throughout this chapter, we call methods for the general oscillatory system (8.1) *general ERKN methods*, and *standard ERKN methods*, for the special case (8.2).

8.3 The Failure and the Reduction of the EN-T Theory

The EN-T theory for general ERKN methods was presented in the recent paper [33] in which some tri-colored trees are supplemented to *the classical Nyström trees* (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 [33] tried to eliminate the difference and then to make one elementary differential correspond to one tree uniquely. Unfortunately, however, the paper [33] did not succeed on this point. For example, the two different trees shown in Table 8.1 have the same elementary differentials $\mathscr{F}(\tau)(\boldsymbol{y}, \boldsymbol{y}')$.

Moreover, the great limitation of the EN-T theory is the existence of great numbers of redundant trees that cause trouble in applications. For example, in Table 8.2 (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 (8.4).

Here, it should be pointed out that it is not necessary that one tree corresponds to one elementary differential. In other words, one tree may correspond to a set

Table 8.1 Two EN-Ts which have the same elementary differentials $\mathscr{F}(\tau)(\boldsymbol{y}, \boldsymbol{y}')$

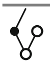
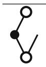
EN-Ts	ρ	γ	Φ_i	α	$\mathscr{F}$
	4	4	$c_i^2 \sum_j a_{ij}^{(0)}$	3	$\boldsymbol{f}_{\boldsymbol{y}\boldsymbol{y}'}^{(2)}(-M\boldsymbol{y}, \boldsymbol{f})$
	4	8	$c_i \sum_j \bar{a}_{ij}^{(0)}$	3	$\boldsymbol{f}_{\boldsymbol{y}\boldsymbol{y}'}^{(2)}(-M\boldsymbol{y}, \boldsymbol{f})$

Table 8.2 Some EN-Ts and the redundance

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

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

of elementary differentials. For example, just as shown in Table 8.2, the sum of the products of the coefficient $\alpha(\tau)$ and the elementary differentials $\mathscr{F}(\tau)(\boldsymbol{y}, \boldsymbol{y}')$ is meaningful. In fact, we have

$$\boldsymbol{f}^{(1)}_{\boldsymbol{y}}\boldsymbol{y}' + \boldsymbol{f}^{(1)}_{\boldsymbol{y}'}(-My) = D^1_h \boldsymbol{f}\Big(\phi_0(h^2M)\boldsymbol{y} + \phi_1(h^2M)h\boldsymbol{y}', \phi_0(h^2M)\boldsymbol{y}' - hM\phi_1(h^2M)\boldsymbol{y}\Big),$$

namely, $\boldsymbol{f}^{(1)}_{\boldsymbol{y}}\boldsymbol{y}' + \boldsymbol{f}^{(1)}_{\boldsymbol{y}'}(-My)$ 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

$$\hat{\boldsymbol{y}} = \phi_0(h^2M)\boldsymbol{y} + \phi_1(h^2M)h\boldsymbol{y}', \tag{8.6}$$

$$\hat{\boldsymbol{y}}' = \phi_0(h^2M)\boldsymbol{y}' - hM\phi_1(h^2M)\boldsymbol{y}. \tag{8.7}$$

Thus, in Table 8.2, we can choose these two bi-colored trees to respectively represent the sums, and omit all trees with meagre vertices. In this way, we can get rid of the redundance as shown in Table 8.2 (right).

On the other hand, although almost all tri-colored trees are redundant, there indeed exist tri-colored trees which are absolutely necessary in the research of order conditions for the general ERKN methods (8.4). For example, the fifth tree which is tri-colored in the fifth line in the Table 2 in [33] undoubtedly works for the order conditions. In a word, the theory for the general ERKN methods (8.4) is a tri-colored tree theory, but it is based on a subset of the EN-T set.

Hence, it is quite natural that this chapter starts from the Nth 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 [1, 30]. In what follows we will denote this derivative as $D_h^N\boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m\boldsymbol{y}'^n}$.

Remark 8.1 The dimension of the matrix $D_h^N\boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m\boldsymbol{y}'^n}$ is $d\times d^{m+n}$. If $\boldsymbol{z}$ is a $d^{m+n}\times 1$ matrix, the dimension of $D_h^N\boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m\boldsymbol{y}'^n}\boldsymbol{z}$ is $d\times 1$.

Remark 8.2 If the matrix M is null,

$$D_h^N\boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m\boldsymbol{y}'^n}\boldsymbol{z}=\boldsymbol{f}^{(m+n+N)}_{\boldsymbol{y}^{m+N}\boldsymbol{y}'^n}\Big(\underbrace{\boldsymbol{y}',\cdots,\boldsymbol{y}'}_{N\text{ fold}},\boldsymbol{z}\Big),$$

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 [30]).

Remark 8.3 In the special case (8.2) where the function $\boldsymbol{f}$ is independent of $\boldsymbol{y}'$, $D_h^N\boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m\boldsymbol{y}'^n}\boldsymbol{z}$ is exactly $D_h^N\boldsymbol{f}^{(m)}\boldsymbol{z}$ in [30].

At the end of this section we give the following first three results of $D_h^N\boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m\boldsymbol{y}'^n}\boldsymbol{z}$, which contribute significantly to our understanding of the extended elementary differentials (see Definition 8.3 in Sect. 8.4).

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

Table 8.3 Four theory systems for second order differential equations

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

8.4 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 8.3, where the abbreviation "SSEN-T" is for *simplified special extended Nyström-tree* [30], and here the word "compact" should be interpreted as meaning that any order condition derived from a tree belonging the underlining rooted tree set cannot be obtained by another from the same rooted tree set.

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

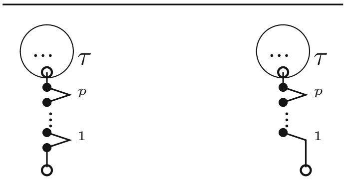
Moreover, when the matrix M is null, the third is identical to the first, and the fourth to the second. In a word, the last two systems are the extensions of the first two systems respectively. However, the extension of the first system is not satisfied yet, since the last section in this chapter states that the third 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-colored rooted tree set and six mappings onto it. In this section, we will define the new tree set and study the relationships to the N-T set, the EN-T set, and the SSEN-T set.

8.4.1 The IEN-T Set and the Related Mappings

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

Definition 8.2 The improved extended-Nyström tree (IEN-T) set, is recursively defined as follows:

Table 8.4 Tree $W_+B_+(b_+B_+)^p(\tau)$ (left), and tree $W_+(b_+B_+)^p(\tau)$ (right) in Definition 8.2



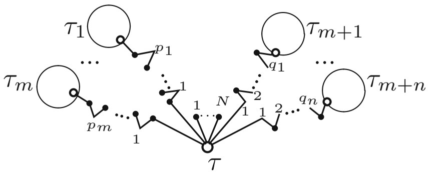
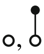


Fig. 8.1 The mode of the trees in the IEN-T set

(a)  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 8.4), 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 8.4), belongs to the IEN-T set for $\forall p = 0, 1, 2, \ldots$.

(d) If $\tau_1, \ldots, \tau_\mu$ 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 [4].

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

$$\tau := \underbrace{\tau_* \times \cdots \times \tau_*}_{N-\text{fold}} \times \Big(W_+B_+(b_+B_+)^{p_1}(\tau_1)\Big) \times \cdots \times \Big(W_+B_+(b_+B_+)^{p_m}(\tau_m)\Big) \times \Big(W_+(b_+B_+)^{q_1}(\tau_{m+1})\Big) \times \cdots \times \Big(W_+(b_+B_+)^{q_n}(\tau_{m+n})\Big), \tag{8.8}$$

where $\tau_* =$ . Figure 8.1 gives the mode of the trees in the IEN-T set.

On the basis of Definition 8.2, 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.
(iv) A meagre vertex must has one fat black vertex as its child, and must have a white vertex as its descendant.

Definition 8.3 The order $\rho(\tau)$, the extended elementary differential $\mathscr{F}(\tau)(\boldsymbol{y}, \boldsymbol{y}')$, the coefficient $\alpha(\tau)$, 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. $\rho(\circ) = 1$, $\mathscr{F}(\circ) = \boldsymbol{f}$, $\alpha(\circ) = 1$, $\Phi_i(\circ) = 1$, $\gamma(\circ) = 1$ and $S(\circ) = 1$.
2. For $\tau \in$ IEN-T denoted by (8.8),
   - $\rho(\tau) = 1 + N + \sum\limits_{i=1}^{m}\Big(1 + 2p_i + \rho(\tau_i)\Big) + \sum\limits_{i=1}^{n}\Big(2q_i + \rho(\tau_{m+i})\Big)$,
   - $\mathscr{F}(\tau) = D_h^N \boldsymbol{f}_{\boldsymbol{y}^m \boldsymbol{y}'^n}^{(m+n)}\Big((-M)^{p_1}\mathscr{F}(\tau_1), \cdots, (-M)^{p_{m+n}}\mathscr{F}(\tau_{m+n})\Big)$,

     where $p_{m+i} = q_i, i = 1, \cdots, n$, and $(\cdot, \cdots, \cdot)$ is the Kronecker inner product (see [30]),
   - $\alpha(\tau) = (\rho(\tau) - 1)! \cdot \frac{1}{N!} \cdot \prod\limits_{i=1}^{m}\Big(\frac{\alpha(\tau_i)}{(1+2p_i+\rho(\tau_i))!}\Big) \cdot \prod\limits_{i=1}^{n}\Big(\frac{\alpha(\tau_{m+i})}{(2q_i+\rho(\tau_{m+i}))!}\Big) \cdot \frac{1}{J_1!\ldots J_I!}$,

     where $J_1, \cdots, J_I$ count the same branches,
   - $\Phi_i(\tau) = c_i^N \cdot \prod\limits_{k=1}^{m}\Big(\sum\limits_{j=1}^{s} \bar{a}_{ij}^{(2p_k)}\Phi_j(\tau_k)\Big) \cdot \prod\limits_{k=1}^{n}\Big(\sum\limits_{j=1}^{s} a_{ij}^{(2q_k)}\Phi_j(\tau_{m+k})\Big)$,
   - $\gamma(\tau) = \rho(\tau) \cdot \prod\limits_{i=1}^{m}\Big(\frac{(1+2p_i+\rho(\tau_i))!\gamma(\tau_i)}{(2p_i)!\rho(\tau_i)!}\Big) \cdot \prod\limits_{i=1}^{n}\Big(\frac{(2q_i+\rho(\tau_{m+i}))!\gamma(\tau_{m+i})}{(2q_i)!\rho(\tau_{m+i})!}\Big)$,
   - $S(\tau) = \prod\limits_{i=1}^{m}\Big((-1)^{p_i}S(\tau_i)\Big) \cdot \prod\limits_{i=1}^{n}\Big((-1)^{q_i}S(\tau_{m+i})\Big)$,

where $\sum\limits_{k=1}^{0} = 0$ and $\prod\limits_{k=1}^{0} = 1$.

Definition 8.4 The set IEN-T$_m$ is defined as

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

Remark 8.4 The order $\rho(\tau)$ is the number of the tree τ's vertices.

Remark 8.5 The extended elementary differential $\mathscr{F}(\tau)$ is a product of $(-M)^p$ (p is the number of meagre vertices between a white vertex and the next coming white vertex), and $D_h^N \boldsymbol{f}_{\boldsymbol{y}^m \boldsymbol{y}'^n}^{(n+m)}$ (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 8.6 One IEN-T corresponds to one extended elementary differential $\mathscr{F}(\tau)$.

Remark 8.7 The coefficient $\alpha(\tau)$ is the number of possible different monotonic labelings of τ.

Remark 8.8 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 8.9 One IEN-T corresponds to one weight $\Phi_i(\tau)$.

Remark 8.10 The density $\gamma(\tau)$ is the product of the density of a tree by overlooking the differences between vertices, and $\frac{1}{(2p)!}$, where p is the number of the meagre vertices between two white vertices.

Remark 8.11 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 8.5 makes a list of the corresponding mappings: the order ρ, the sign S, the density γ, the weight Φ_i, the symmetry α and the extended elementary differential $\mathscr{F}$ for each τ in the IEN-T set of order up to 4.

8.4.2 *The IEN-T Set and the N-T Set*

In this subsection, we will 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 form shown in Fig 8.2, and the rules to form the tree set are straightforwardly reduced to:

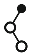
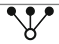
(i) The root of a tree is always a fat white vertex.
(ii) A white vertex has fat black children, or white children.
(iii) A fat black vertex has at most one child which must be white.

In this case, from Remarks 8.4–8.10, the order $\rho(\tau)$, the coefficient $\alpha(\tau)$ 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 $\mathscr{F}(\tau)(\boldsymbol{y}, \boldsymbol{y}')$ on the IEN-T set are exactly the same as the ones on the N-T set respectively, too. In fact, from Definition 8.3, with the disappearance of meagre vertices, these two mappings are recursively defined respectively, for τ denoted by Fig. 8.2, as follows:

$$\Phi_i(\tau) = c_i^N \cdot \prod_{k=1}^{m}\Big(\sum_{j=1}^{s} \bar{a}_{ij}\Phi_j(\tau_k)\Big) \cdot \prod_{k=1}^{n}\Big(\sum_{j=1}^{s} a_{ij}\Phi_j(\tau_{m+k})\Big),$$

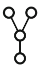
$$\mathscr{F}(\tau) = D_h^N \boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m \boldsymbol{y}'^n}\Big(\mathscr{F}(\tau_1), \cdots, \mathscr{F}(\tau_{m+n})\Big).$$

Table 8.5 IEN-Ts and mappings of order up to 4 and the corresponding elementary differentials on the N-T set

No.	IEN-Ts	ρ	S	γ	Φ_i	α	$\mathscr{F}$	$\mathscr{F}$ 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	$\boldsymbol{f}_{\boldsymbol{y}'\boldsymbol{y}'}^{(2)}(\boldsymbol{f}, D_h^1 \boldsymbol{f})$	$f''_{y'y'}(f_y y', f)$

(continued)

Table 8.5 (continued)

No.	IEN-Ts	ρ	S	γ	Φ_i	α	$\mathscr{F}$	$\mathscr{F}$ on the N-T set
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	$\boldsymbol{f}_{\boldsymbol{y}'}^{(1)} \boldsymbol{f}_{\boldsymbol{y}}^{(1)} \boldsymbol{f}$	$f'_{y'} f'_y f$
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	c_i	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	$\boldsymbol{f}_{\boldsymbol{y}'}^{(1)} \boldsymbol{f}_{\boldsymbol{y}'\boldsymbol{y}'}^{(2)} (\boldsymbol{f}, \boldsymbol{f})$	$f'_{y'} f''_{y'y'}(f, f)$

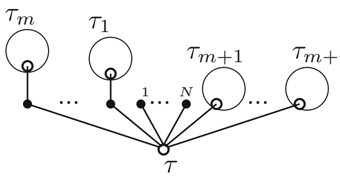
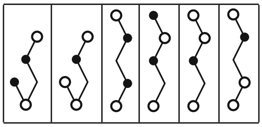


Fig. 8.2 The form of the trees with meagre vertices disappearing

Table 8.6 Tri-colored 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 [4]). It can also be seen from Tables 8.5 and 8.6 that one 4th order tree, 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 8.6 are all the functions of $\bar{a}_{ij}^{(2k)}$ and $a_{ij}^{(2k)}$, high-order derivatives of $\bar{a}_{ij}(V)$ and $a_{ij}(V)$ with respect to h, at $h = 0$.

8.4.3 The IEN-T Set and the EN-T Set

First of all, we note that there are just five mappings defined on the EN-T set in the paper [33], while there are six mappings on the IEN-T set in this chapter. In the paper [33], the authors introduced *the signed density* $\tilde{\gamma}(\tau)$, but in this chapter 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 $\mathscr{F}(\tau)$ on them.

8.4.4 The IEN-T Set and the SSEN-T Set

From the rules of the IEN-T set and of the SSEN-T set (see [30]), if the function $\boldsymbol{f}$ in the system (8.1) does not containing $\boldsymbol{y}'$ explicitly, the IEN-T set is exactly the SSEN-T set.

8.5 B-Series for the General ERKN Method

In Sect. 8.4 we presented the IEN-T set, on which six mappings are defined. With these preliminaries, motivated by the concept of B-series, we will describe a totally different approach from the one described in [33] 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 [2] of Butcher in 1972, and then are introduced in detail by Hairer and Wanner [5] in 1974. In what follows, we present the following two elementary theorems.

Theorem 8.1 *With Definition 8.3, $\boldsymbol{f}(\boldsymbol{y}(t+h), \boldsymbol{y}'(t+h))$ is a B-series*

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

Proof First, we expand $\boldsymbol{f}(\boldsymbol{y}(t+h), \boldsymbol{y}'(t+h))$ at point $(\hat{\boldsymbol{y}}, \hat{\boldsymbol{y}}')$, with the definitions of (8.6) and (8.7).

$$\boldsymbol{f}(\boldsymbol{y}(t+h), \boldsymbol{y}'(t+h)) = \sum_{m \geq 0, n \geq 0} \frac{1}{(m+n)!} \boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m \boldsymbol{y}'^n}\Big|_{(\hat{\boldsymbol{y}}, \hat{\boldsymbol{y}}')} \Big(\boldsymbol{y}(t+h) - \hat{\boldsymbol{y}}\Big)^{\otimes m} \otimes \Big(\boldsymbol{y}'(t+h) - \hat{\boldsymbol{y}}'\Big)^{\otimes n}, \tag{8.9}$$

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 8.3 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 [33]), and from the properties of the ϕ-functions (see e.g. [25]), we have

$$\begin{aligned} \boldsymbol{y}(t+h) - \hat{\boldsymbol{y}} &= h^2 \int_0^1 (1-z)\phi_1((1-z)^2 V) \boldsymbol{f}(\boldsymbol{y}(t+hz), \boldsymbol{y}'(t+hz)) \mathrm{d}z \\ &= \sum_{\tau \in \mathrm{IEN-T}} \int_0^1 (1-z)\phi_1((1-z)^2 V) \tfrac{z^{\rho(\tau)-1}}{(\rho(\tau)-1)!} \mathrm{d}z \cdot \Big(h^{\rho(\tau)+1} \alpha(\tau) \mathscr{F}(\tau)(\boldsymbol{y}, \boldsymbol{y}')\Big) \\ &= \sum_{\tau \in \mathrm{IEN-T}} \phi_{\rho(\tau)+1}(V) \cdot h^{\rho(\tau)+1} \alpha(\tau) \mathscr{F}(\tau)(\boldsymbol{y}, \boldsymbol{y}') \\ &= \sum_{\tau \in \mathrm{IEN-T}} \sum_{p \geq 0} \tfrac{(-1)^p V^p}{(\rho(\tau)+1+2p)!} h^{\rho(\tau)+1} \alpha(\tau) \mathscr{F}(\tau)(\boldsymbol{y}, \boldsymbol{y}'), \end{aligned} \tag{8.10}$$

and

$$\boldsymbol{y}'(t+h) - \hat{\boldsymbol{y}}' = \sum_{\tau \in \mathrm{IEN-T}} \sum_{q \geq 0} \tfrac{(-1)^q V^q}{(\rho(\tau)+2q)!} h^{\rho(\tau)} \alpha(\tau) \mathscr{F}(\tau)(\boldsymbol{y}, \boldsymbol{y}'). \tag{8.11}$$

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 (8.10) and (8.11), the Eq. (8.9) becomes

$$\begin{aligned} \boldsymbol{f}(\boldsymbol{y}(t+h), \boldsymbol{y}'(t+h)) = \sum_{N,n,m} \sum_{\tau \in \mathrm{IEN-T}} \tfrac{h^s}{N!(m+n)!} D_h^N \boldsymbol{f}^{(n+m)}_{\boldsymbol{y}^m \boldsymbol{y}'^n} \Big(\tfrac{(-M)^{p_1} \alpha(\tau_1) \mathscr{F}(\tau_1)(\boldsymbol{y})}{(\rho(\tau_1)+1+2p_1)!}, \ldots, \\ \tfrac{(-M)^{p_m} \alpha(\tau_m) \mathscr{F}(\tau_m)(\boldsymbol{y})}{(\rho(\tau_m)+1+2p_m)!}, \tfrac{(-M)^{q_1} \alpha(\tau_{m+1}) \mathscr{F}(\tau_{m+1})(\boldsymbol{y})}{(\rho(\tau_{m+1})+2q_1)!}, \ldots, \tfrac{(-M)^{q_n} \alpha(\tau_{m+n}) \mathscr{F}(\tau_{m+n})(\boldsymbol{y})}{(\rho(\tau_{m+n})+2q_n)!} \Big), \end{aligned} \tag{8.12}$$

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 8.3, the proof is complete.

Theorem 8.2 *Given a general ERKN method (8.4), by Definition 8.3, each $\boldsymbol{f}(Y_i, Y_i')$ is a series of the form*

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

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

Proof In a similar way to the proof of Theorem 8.1, we expand $\boldsymbol{f}(Y_i, Y_i')$ at $(\tilde{\boldsymbol{y}}, \tilde{\boldsymbol{y}}')$ for the general ERKN method (8.4), 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:

$$\boldsymbol{f}(Y_i, Y_i') = \sum_{m,n \geq 0} \frac{1}{(m+n)!} \boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m \boldsymbol{y}'^n}\Big|_{\tilde{\boldsymbol{y}}, \tilde{\boldsymbol{y}}'} \Big(h^2 \sum_j \bar{a}_{ij}(V)\boldsymbol{f}(Y_j, Y_j')\Big)^{\otimes m} \otimes \Big(h \sum_j a_{ij}(V)\boldsymbol{f}(Y_j, Y_j')\Big)^{\otimes n}, \tag{8.13}$$

where the second term $\boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m \boldsymbol{y}'^n}\Big|_{\tilde{\boldsymbol{y}}, \tilde{\boldsymbol{y}}'}$ is a 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

$$\boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m \boldsymbol{y}'^n}\Big|_{(\hat{\boldsymbol{y}}, \hat{\boldsymbol{y}}')} = \sum_{N \geq 0} \frac{c_i^N}{m!} h^N D_h^N \boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m \boldsymbol{y}'^n}. \tag{8.14}$$

Definition 8.3 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 Eq. (8.13) are given by

$$h^2 \textstyle\sum_j \bar{a}_{ij}(V)\boldsymbol{f}(Y_j, Y_j') = \displaystyle\sum_{\tau \in \mathrm{IEN-T}} \sum_{p \geq 0} \frac{\sum_j \bar{a}_{ij}^{(2p)}}{\rho(\tau)!} \frac{V^p}{(2p)!} h^{\rho(\tau)+1} \boldsymbol{a}_j(\tau), \tag{8.15}$$

and

$$h \textstyle\sum_j a_{ij}(V)\boldsymbol{f}(Y_j, Y_j') = \displaystyle\sum_{\tau \in \mathrm{IEN-T}} \sum_{q \geq 0} \frac{\sum_j a_{ij}^{(2q)}}{\rho(\tau)!} \frac{V^q}{(2q)!} h^{\rho(\tau)} \boldsymbol{a}_j(\tau). \tag{8.16}$$

We then obtain

$$\begin{aligned}\boldsymbol{f}(Y_i, Y_i') = \sum_{N,n,m} \sum_{\tau \in \mathrm{IEN-T}} \frac{c_i^N h^s}{N!(n+m)!} D_h^N \boldsymbol{f}^{(m+n)}_{\boldsymbol{y}^m \boldsymbol{y}'^n} \Big(&\frac{\sum_j \bar{a}_{ij}^{(2p_1)}}{\rho(\tau_1)!} \frac{M^{p_1}}{(2p_1)!} \boldsymbol{a}_j(\tau_1), \ldots, \frac{\sum_j \bar{a}_{ij}^{(2p_m)}}{\rho(\tau_m)!} \frac{M^{p_m}}{(2p_m)!} \boldsymbol{a}_j(\tau_m), \\ &\frac{\sum_j a_{ij}^{(2q_1)}}{\rho(\tau_{m+1})!} \frac{M^{q_1}}{(2q_1)!} \boldsymbol{a}_j(\tau_{m+1}), \ldots, \frac{\sum_j a_{ij}^{(2q_n)}}{\rho(\tau_{m+n})!} \frac{M^{q_n}}{(2q_n)!} \boldsymbol{a}_j(\tau_{m+n}) \Big),\end{aligned} \tag{8.17}$$

where $s = N + \sum_{k=1}^{m}(2p_k + \rho(\tau_k) + 1) + \sum_{k=1}^{n}(2q_k + \rho(\tau_{m+k}))$. Using Definition 8.3, we complete the proof.

8.6 The Order Conditions for the General ERKN Method

Theorem 8.3 *The scheme (8.4) for the general multi-frequency and multidimensional oscillatory second-order initial value problems (8.1) has order r if and only if the following conditions*

$$\sum_{i=1}^{s}\bar{b}_i(V)S(\tau)\gamma(\tau)\Phi_i(\tau)=\rho(\tau)!\phi_{\rho(\tau)+1}+O(h^{r-\rho(\tau)}),\quad \forall\tau\in IEN\text{-}T_m,\ m\leq r-1, \tag{8.18}$$

$$\sum_{i=1}^{s}b_i(V)S(\tau)\gamma(\tau)\Phi_i(\tau)=\rho(\tau)!\phi_{\rho(\tau)}+O(h^{r-\rho(\tau)+1}),\quad \forall\tau\in IEN\text{-}T_m,\ m\leq r, \tag{8.19}$$

are satisfied.

Proof It follows from the matrix-variation-of-constants formula, Theorems 8.1 and 8.2 that

$$\begin{aligned}\boldsymbol{y}_{n+1}&=\phi_0(V)\boldsymbol{y}_n+h\phi_1(V)\boldsymbol{y}'_n\\&\quad+\sum_{\tau\in\text{IEN}-\text{T}}\frac{h^{\rho(\tau)+1}}{\rho(\tau)!}\sum_{i=1}^{s}\bar{b}_i(V)\Phi_i(\tau)S(\tau)\gamma(\tau)\alpha(\tau)\mathscr{F}(\tau)(\boldsymbol{y}_n,\boldsymbol{y}'_n),\end{aligned} \tag{8.20}$$

$$\begin{aligned}\boldsymbol{y}(t+h)&=\phi_0(V)\boldsymbol{y}+h\phi_1(V)\boldsymbol{y}'\\&\quad+\sum_{\tau\in\text{IEN-T}}h^{\rho(\tau)+1}\alpha(\tau)\mathscr{F}(\tau)(\boldsymbol{y},\boldsymbol{y})\int_0^1(1-z)\frac{z^{\rho(\tau)-1}}{(\rho(\tau)-1)!}\phi_1((1-z)V)\,\mathrm{d}z.\end{aligned} \tag{8.21}$$

Comparing the Eqs. (8.20) with (8.21) and using the properties of the ϕ-functions, we obtain the first result of Theorem 8.3. Likewise, we deduce the second part of the theorem.

Theorem 8.3 in this chapter and Theorem 4.1 in [33] share the same expression. However, it should be noted that there exist redundant order conditions in [33], while any order condition in this chapter 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 (8.4) are independent. Obviously, the elimination of redundant order conditions makes the construction of high-order general ERKN methods (8.4) much clearer and simpler.

It is easy to see that Theorem 8.3 implies the order conditions for the standard ERKN methods in [23, 30] when the right-hand side function $\boldsymbol{f}$ does not depend on $\boldsymbol{y}'$. It is noted that, if the matrix M is null, Theorem 8.3 reduces to 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.

8.7 The Construction of General ERKN Methods

In this section, using Theorem 8.3, we present some general ERKN methods (8.4) of order up to 4. The approach to constructing new methods in this section is different from that described in [33].

8.7.1 Second-Order General ERKN Methods

From Theorem 8.3 and the three IEN-Ts with order no more than 2 which are listed in Table 8.5, for an s-stage general ERKN method (8.4) expressed in the Butcher tableau (8.5), we have the following second order conditions:

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

Comparing the coefficients of h^0 and h, we obtain 4 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 these equations are exactly the second order conditions for the following traditional RKN method

$$\begin{cases}
Y_i=\boldsymbol{y}_n+c_ih\boldsymbol{y}'_n+h^2\displaystyle\sum_{j=1}^{s}\bar{a}_{ij}^{(0)}\Big(\boldsymbol{f}(Y_j,Y'_j)-MY_j\Big), \qquad i=1,\cdots,s,\\
Y'_i=\boldsymbol{y}'_n+h\displaystyle\sum_{j=1}^{s}a_{ij}^{(0)}\Big(\boldsymbol{f}(Y_j,Y'_j)-MY_j\Big), \qquad i=1,\cdots,s,\\
\boldsymbol{y}_{n+1}=\boldsymbol{y}_n+h\boldsymbol{y}'_n+h^2\displaystyle\sum_{i=1}^{s}\bar{b}_i^{(0)}\Big(\boldsymbol{f}(Y_i,Y'_i)-MY_i\Big),\\
\boldsymbol{y}'_{n+1}=\boldsymbol{y}'_n+h\displaystyle\sum_{i=1}^{s}b_i^{(0)}\Big(\boldsymbol{f}(Y_i,Y'_i)-MY_i\Big),
\end{cases} \tag{8.22}$$

applied to the initial value problems (8.1), with the tableau

$$\begin{array}{c|cccc|cccc} c_1 & \bar{a}_{11}^{(0)} & \bar{a}_{12}^{(0)} & \cdots & \bar{a}_{1s}^{(0)} & a_{11}^{(0)} & a_{12}^{(0)} & \cdots & a_{1s}^{(0)} \\ c_2 & \bar{a}_{21}^{(0)} & \bar{a}_{22}^{(0)} & \cdots & \bar{a}_{2s}^{(0)} & a_{21}^{(0)} & a_{22}^{(0)} & \cdots & a_{2s}^{(0)} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & \bar{a}_{s1}^{(0)} & \bar{a}_{s2}^{(0)} & \cdots & \bar{a}_{s,s}^{(0)} & a_{s1}^{(0)} & a_{s2}^{(0)} & \cdots & a_{s,s}^{(0)} \\ \hline & \bar{b}_1^{(0)} & \bar{b}_2^{(0)} & \cdots & \bar{b}_s^{(0)} & b_1^{(0)} & b_2^{(0)} & \cdots & b_s^{(0)} \end{array}. \tag{8.23}$$

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 second-order general RKN method with the Butcher tableau

$$\begin{array}{c|cc|cc} 0 & & & & \\ \frac{2}{3} & 0 & & \frac{2}{3} & \\ \hline & \frac{1}{4} & \frac{3}{4} & \frac{1}{4} & \frac{1}{4} \end{array}, \tag{8.24}$$

we can obtain 2 stage second-order explicit general ERKN methods. Two examples are given below.

Example 1 The first 2 stage second-order explicit general ERKN method (8.4) has Butcher tableau

$$\begin{array}{c|cc|cc} 0 & & & & \\ \frac{2}{3} & 0 & & \frac{2}{3}I & \\ \hline & \frac{1}{4}I & \frac{3}{4}I & \frac{1}{4}I & \frac{1}{4}I \end{array}. \tag{8.25}$$

Example 2 The Butcher tableau of the second one is

$$\begin{array}{c|cc|cc} 0 & & & & \\ \frac{2}{3} & 0 & & \frac{2}{3}\phi_0(\frac{4}{9}V) & \\ \hline & \frac{1}{4}\phi_1(V) & \frac{3}{4}\phi_1(\frac{1}{9}V) & \frac{1}{4}\phi_0(V) & \frac{1}{4}\phi_0(\frac{1}{9}V) \end{array}. \tag{8.26}$$

8.7.2 Third-Order General ERKN Methods

From Theorem 8.3 and 9 trees in the set of IEN-T$_m$, ($m \le 3$) in Table 8.5, for an s-stage general ERKN method (8.4) expressed in the Butcher tableau (8.5), we have the third order conditions as follows:

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

Equating coefficients for each power of h, we obtain 13 equations, where 12 equations are exactly the third order conditions for the classical general RKN method (8.22) with the Butcher tableau (8.23)

$$\sum_{i=1}^{s} \bar{b}_i^{(0)} \gamma(\tau)\Phi_i(\tau) = \frac{1}{\rho(\tau)+1}, \quad \forall\tau \in \text{N-T}_m,\ m \le 2, \tag{8.27}$$

$$\sum_{i=1}^{s} b_i^{(0)} \gamma(\tau)\Phi_i(\tau) = 1, \quad \forall\tau \in \text{N-T}_m,\ m \le 3. \tag{8.28}$$

The extra equation is $\sum_{i=1}^{s} \bar{b}_i^{(2)} = -\frac{1}{3}$. We can solve $\left(c_i, \bar{a}_{ij}^{(0)}, a_{ij}^{(0)}, \bar{b}_i^{(0)}, b_i^{(0)}\right)$ from the Eqs. (8.27) and (8.28) via a classical general RKN method. We can then find $b_i^{(2)}$ from the extra equation. Using this approach, we can complete the construction of the general ERKN methods of order three. For example, from the explicit 3 stage third-order general RKN method with the Butcher tableau

$$\begin{array}{c|ccc|ccc} 0 & & & & & & \\ \frac{1}{2} & 0 & & & \frac{1}{2} & & \\ 1 & 1 & 0 & & -1 & 2 & \\ \hline & \frac{1}{6} & \frac{2}{6} & 0 & \frac{1}{6} & \frac{4}{6} & \frac{1}{6} \end{array} \tag{8.29}$$

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

Example 3 The first 3 stage third-order explicit general ERKN method (8.4) is expressed in the Butcher tableau

$$\begin{array}{c|ccc|ccc} 0 & & & & & & \\ \frac{1}{2} & 0 & & & \frac{1}{2}I & & \\ 1 & I & 0 & & -I & 2I & \\ \hline & \frac{1}{6}I & \frac{2}{6}I & 0 & \frac{1}{6}(I-\frac{9}{20}V) & \frac{4}{6}(I-\frac{3}{20}V) & \frac{1}{6}(I+\frac{1}{20}V) \end{array}. \tag{8.30}$$

Example 4 The Butcher tableau of the second 3 stage third-order explicit general ERKN method (8.4) is given by

$$\begin{array}{c|ccc|ccc} 0 & & & & & & \\ \frac{1}{2} & 0 & & & \frac{1}{2}I & & \\ 1 & I & 0 & & -I & 2I & \\ \hline & \frac{1}{6}(I-\frac{1}{6}V) & \frac{2}{6}(I-\frac{1}{24}V) & 0 & \frac{1}{6}(I-\frac{1}{2}V) & \frac{4}{6}(I-\frac{1}{8}V) & \frac{1}{6}I \end{array}. \tag{8.31}$$

Example 5 The third 3 stage third-order explicit general ERKN method (8.4) is denoted by the Butcher tableau

$$\begin{array}{c|ccc|cccc} 0 & & & & & & & \\ \frac{1}{2} & 0 & & & \frac{1}{2}\phi_0(\frac{1}{4}V) & & & \\ 1 & \phi_1(V) & 0 & & -\phi_0(V) & 2\phi_0(\frac{1}{4}V) & & \\ \hline & \frac{1}{6}\phi_1(V) & \frac{2}{6}\phi_1(\frac{1}{4}V) & 0 & \frac{1}{6}\phi_0(V) & \frac{4}{6}\phi_0(\frac{1}{4}V) & \frac{1}{6}I \end{array} \,. \tag{8.32}$$

8.7.3 Fourth-Order General ERKN Methods

From Theorem 8.3 and Table 8.5, comparing the coefficients of the power of h of (8.18) and (8.19), for an s-stage general ERKN method (8.4) with the coefficient $\left(\bar{a}_{ij}(V), a_{ij}(V), \bar{b}_i(V), b_i(V)\right)$ displayed in the Butcher tableau (8.5), we can obtain 41 fourth order conditions, in which 36 conditions are as follows:

$$\sum_{i=1}^{s} \bar{b}_i^{(0)} \gamma(\tau) \Phi_i(\tau) = \frac{1}{\rho(\tau)+1}, \quad \forall \tau \in \text{N-T}_m,\ m \le 3, \tag{8.33}$$

$$\sum_{i=1}^{s} b_i^{(0)} \gamma(\tau) \Phi_i(\tau) = 1, \quad \forall \tau \in \text{N-T}_m,\ m \le 4. \tag{8.34}$$

The remaining 5 conditions are

$$\begin{aligned} &\sum_{i=1}^{s}\sum_{j=1}^{s} b_i^{(0)} a_{ij}^{(2)} = -\frac{1}{12},\ \sum_{i=1}^{s} b_i^{(2)} = -\frac{1}{3},\ \sum_{i=1}^{s} b_i^{(2)} c_i = -\frac{1}{12},\\ &\sum_{i=1}^{s}\sum_{j=1}^{s} b_i^{(2)} a_{ij}^{(0)} = -\frac{1}{12},\ \sum_{i=1}^{s} \bar{b}_i^{(2)} = -\frac{1}{12}. \end{aligned} \tag{8.35}$$

For each specific classical general RKN method of order four, we can solve for $\left(c_i, \bar{a}_{ij}^{(0)}, a_{ij}^{(0)}, \bar{b}_i^{(0)}, b_i^{(0)}\right)$ from (8.33) and (8.34), since these 36 conditions are exactly the order conditions for the classical general RKN method (8.22) with the Butcher tableau (8.23). Then we can find $\left(a_{ij}^{(2)}, \bar{b}_i^{(2)}, b_i^{(2)}\right)$ from conditions (8.35). In this way, we construct the general ERKN methods (8.4) of order four.

In what follows, we will construct explicit 4 stage fourth order general ERKN methods from the following explicit 4 stage fourth-order classical general RKN method (8.22) with the Butcher tableau

$$\begin{array}{c|cccc|cccc} 0 & & & & & & & & \\ \frac{1}{2} & \frac{1}{8} & & & & \frac{1}{2} & & & \\ \frac{1}{2} & \frac{1}{8} & 0 & & & 0 & \frac{1}{2} & & \\ 1 & 0 & 0 & \frac{1}{2} & & 0 & 0 & 1 & \\ \hline & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & 0 & \frac{1}{6} & \frac{2}{6} & \frac{2}{6} & \frac{1}{6} \end{array} \,. \tag{8.36}$$

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 fourth-order general ERKN method (8.4) is given by

$$
\begin{array}{c|cccc|cccc}
0 & & & & & & & & \\
\frac{1}{2} & \frac{1}{8}I & & & & \frac{1}{2}I & & & \\
\frac{1}{2} & \frac{1}{8}I & 0 & & & 0 & \frac{1}{2}I & & \\
1 & 0 & 0 & \frac{1}{2}I & & 0 & 0 & I-\frac{1}{4}V & \\
\hline
 & \frac{1}{6}(I-\frac{1}{12}V) & \frac{1}{6}(I-\frac{1}{12}V) & \frac{1}{6}(I-\frac{1}{12}V) & 0 & \frac{1}{6}(I-\frac{1}{2}V) & \frac{2}{6}(I-\frac{1}{8}V) & \frac{2}{6}(I-\frac{1}{8}V) & \frac{1}{6}I
\end{array}
\quad . \tag{8.37}
$$

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

$$
\begin{array}{c|cccc|cccc}
0 & & & & & & & & \\
\frac{1}{2} & \frac{1}{8}I & & & & \frac{1}{2}(I-\frac{1}{8}V) & & & \\
\frac{1}{2} & \frac{1}{8}I & 0 & & & 0 & \frac{1}{2}I & & \\
1 & 0 & 0 & \frac{1}{2}I & & 0 & 0 & I-\frac{1}{8}V & \\
\hline
 & \frac{1}{6}(I-\frac{1}{6}V) & \frac{1}{6}(I-\frac{1}{24}V) & \frac{1}{6}(I-\frac{1}{24}V) & 0 & \frac{1}{6}(I-\frac{1}{2}V) & \frac{2}{6}(I-\frac{1}{8}V) & \frac{2}{6}(I-\frac{1}{8}V) & \frac{1}{6}I
\end{array}
\quad . \tag{8.38}
$$

Example 8 The third explicit 4 stage fourth-order general ERKN method (8.4) has the Butcher tableau as follows:

$$
\begin{array}{c|cccc|cccc}
0 & & & & & & & & \\
\frac{1}{2} & \frac{1}{8}\phi_1(\frac{1}{4}V) & & & & \frac{1}{2}\phi_0(\frac{1}{4}V) & & & \\
\frac{1}{2} & \frac{1}{8}\phi_1(\frac{1}{4}V) & 0 & & & 0 & \frac{1}{2}I & & \\
1 & 0 & 0 & \frac{1}{2}\phi_1(\frac{1}{4}V) & & 0 & 0 & \phi_0(\frac{1}{4}V) & \\
\hline
 & \frac{1}{6}\phi_1(V) & \frac{1}{6}\phi_1(\frac{1}{4}V) & \frac{1}{6}\phi_1(\frac{1}{4}V) & 0 & \frac{1}{6}\phi_0(V) & \frac{2}{6}\phi_0(\frac{1}{4}V) & \frac{2}{6}\phi_0(\frac{1}{4}V) & \frac{1}{6}I
\end{array}
\quad . \tag{8.39}
$$

8.7.4 An Effective Approach to Constructing the General ERKN Methods

In the paper [33], in order to construct 4th order general ERKN methods for the systems (8.1), the authors first considered all 62 graphs of the EN-Ts (see Tables 1 and 2 in [33]), and then selected and deleted 34 redundant trees. Finally, they obtained 28 non-redundant EN-Ts (see Tables 3 and 4 in [33]). With these 28 EN-Ts, the authors in [33] achieved special 4th-order conditions, and then the authors derived a 4th-order ERKN method under two auxiliary simplifying assumptions.

Obviously, as shown in the paper [33] more than half of the construction effort was spent on drawing the redundant trees. In a word, the process described in the paper [33] is difficult to follow since the number of the redundant trees in the EN-T set is large.

However, in this chapter, these 28 trees can be directly obtained since 27 of them are exactly the classical N-Ts as shown in Sect. 8.4.2. In this way, it becomes quite easy to get the 4th-order conditions for the general ERKN method (8.4). Then using expansions of these order conditions, and equating each power of h, we can see that most are exactly the order conditions for the classical general RKN method (8.22). This approach to constructing the general ERKN integrators is very effective and efficient in practice, as shown in the previous sections where 2nd, 3rd and 4th order general ERKN methods are constructed as examples.

8.8 Numerical Experiments

In this section, some numerical experiments are implemented to illustrate the potential of the general ERKN methods (8.4) 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 ($\log_{10} \|MGE\|$) versus the base-2 logarithm of the stepsizes ($\log_2(h)$). The following 11 methods are used to solve the general system (8.1) for the comparison:

- RKN2: The 2 stage second-order general RKN method (8.24).
- ERKN2a: The first 2 stage second-order general ERKN method (8.25) given in Sect. 8.7 of this chapter.
- ERKN2b: The second 2 stage second-order general ERKN method (8.26) given in Sect. 8.7 of this chapter.
- RKN3: The 3 stage third-order general RKN method (8.29).
- ERKN3a: The first 3 stage third-order general ERKN method (8.30) given in Sect. 8.7 of this chapter.
- ERKN3b: The second 3 stage third-order general ERKN method (8.31) given in Sect. 8.7 of this chapter.
- ERKN3c: The third 3 stage third-order general ERKN method (8.32) given in Sect. 8.7 of this chapter.
- RKN4: The 4 stage fourth-order general RKN method (8.36).
- ERKN4a: The first 4 stage fourth-order general ERKN method (8.37) given in Sect. 8.7 of this chapter.
- ERKN4b: The second 4 stage fourth-order general ERKN method (8.38) given in Sect. 8.7 of this chapter.
- ERKN4c: The third 4 stage fourth-order general ERKN method (8.39) given in Sect. 8.7 of this chapter.

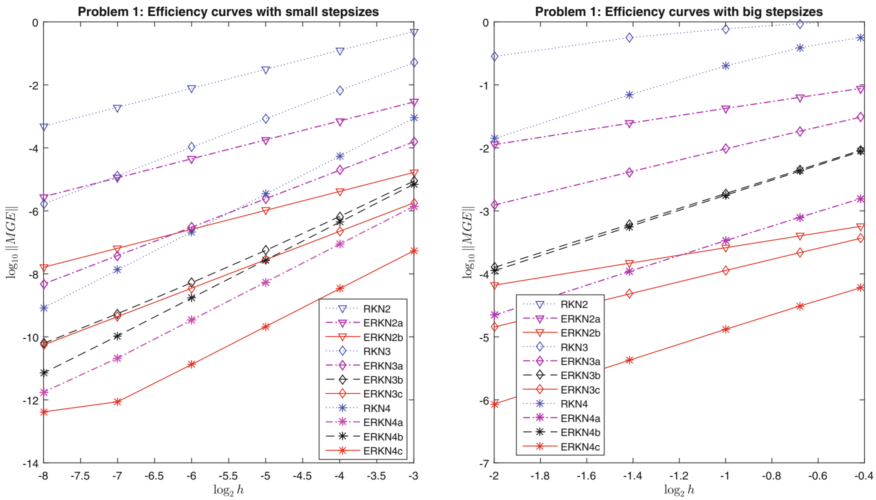


Fig. 8.3 Problem 1 integrated on [0, 300]

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 $\big(y(0), y'(0)\big) = \big(1, 0\big)$. The analytic solution to the problem is given by

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

The numerical results are displayed in Fig. 8.3, 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

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

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

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

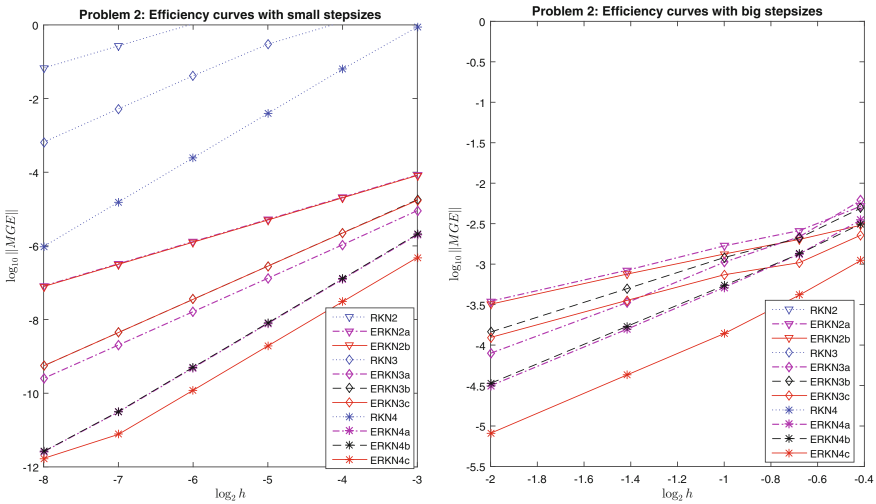


Fig. 8.4 Problem 2 integrated on [0, 300]

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. 8.4. The small stepsizes are $h = \frac{1}{2^j}$ for $j = 3, \ldots, 8$ and the big stepsizes are $h = \frac{j}{8}$ for $j = 2, \ldots, 6$. In this numerical test with the big stepsizes, the classical general RKN methods (RKN2, RKN3 and RKN4) give disappointing numerical results. Thus we do not depict the corresponding points in Fig. 8.4.

Problem 3 Consider the damped wave equation with periodic conditions (wave propagation in a medium, see e.g. Weinberger [18])

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

where $f(u) = -\sin u$, (i.e., 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 $U(t) = \big(u_1(t), \cdots, u_N(t)\big)^{\intercal}$ with $u_i(t) \approx u(x_i, t)$ for $i = 1, \ldots, N$,

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

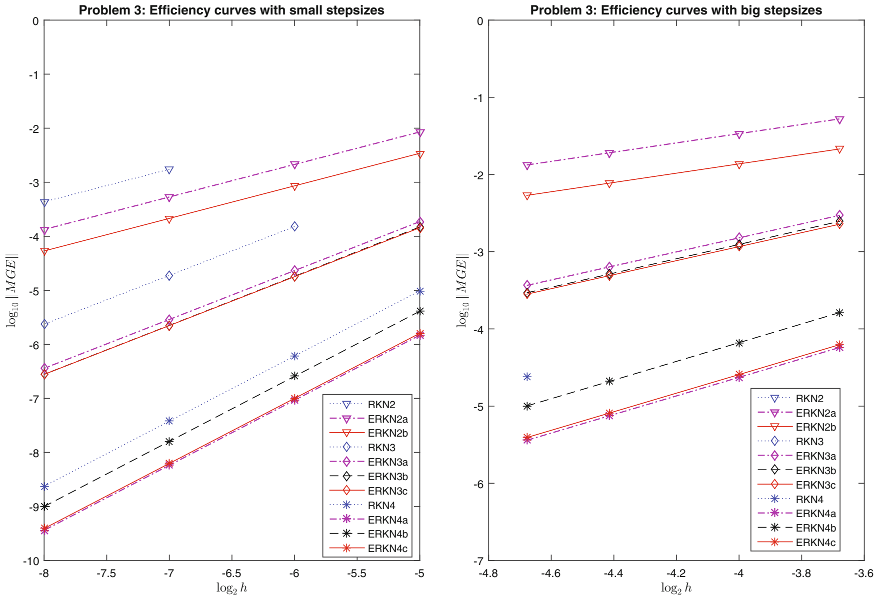


Fig. 8.5 Problem 3 integrated on [0, 300]

$\triangle x = 2/N$, $x_i = -1 + i\triangle x$ and $F(U, \dot{U}) = \big(f(u_1) - \delta\dot{u}_1, \cdots, f(u_N) - \delta\dot{u}_N\big)^{\intercal}$. Following the paper [3], we take the initial conditions as

$$U(0) = \big(\pi, \cdots, \pi\big)^{\intercal}, \quad U_t(0) = \sqrt{N}\Big(0.01 + \sin\big(\frac{2\pi}{N}\big), \cdots, 0.01 + \sin\big(\frac{2\pi N}{N}\big)\Big)^{\intercal},$$

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. 8.5. In this numerical test for the big stepsizes, the classical general RKN methods (RKN2, RKN3 and RKN4) all behave badly, yielding large errors.

It can be observed from Figs. 8.3, 8.4 and 8.5 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.

8.9 Conclusions and Discussions

In this chapter, we have established an improved theory for the order conditions for the general ERKN methods designed specially for solving multi-frequency oscillatory system (8.1). The original tri-colored tree theory and the order conditions for the general ERKN methods presented in the paper [33] are not satisfied yet due to the existence of large numbers of redundant trees. This chapter has succeeded in making a simplification, by defining the IEN-T set 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 (8.1) is of great importance. The new tri-colored tree theory and the B-series theory for the general ERKN methods when solving the general system (8.1) reduce to those for standard ERKN methods when solving special system (8.2), where the right-hand side vector-valued function $\boldsymbol{f}$ does not depend on $\boldsymbol{y}'$ (see [23, 30]).

This successful simplification makes the construction of the general ERKN methods much simpler and more efficient for the system (8.1). In light of the reduced tree theory analysed in this chapter, almost one half of algebraic conditions in the paper [33] can be eliminated. Furthermore, in this chapter, from the relation between the theories of order conditions for the general RKN method and for general ERKN method, we propose a simple approach to constructing 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.

The previous eight chapters concentrated on numerical integrators of oscillatory ordinary differential equations, although their applications to partial differential equations were implemented as well. However, in the next four chapters we will turn to structure-preserving schemes for partial differential equations.

The material of this chapter is based on the work by Zeng et al. [34].

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