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Error bounds for explicit ERKN integrators for systems of multi-frequency oscillatory second-order differential equations ☆

Bin Wang [a], Xinyuan Wu [a,*], Jianlin Xia [b]

[a] *Department of Mathematics, Nanjing University; State Key Laboratory for Novel Software Technology at Nanjing University, Nanjing 210093, PR China*

[b] *Department of Mathematics, Purdue University, West Lafayette, IN 47907, USA*

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ABSTRACT

A substantial issue of numerical analysis is concerned with the investigation and estimation of the errors. In this paper, we pay attention to the error analysis for the extended Runge–Kutta–Nyström (ERKN) integrators proposed by Wu et al. (2010) [30] for systems of multi-frequency oscillatory second-order differential equations $q''(t) + Mq(t) = f(q(t))$. The ERKN integrators are important generalizations of the classical Runge–Kutta–Nyström methods in the sense that both the updates and internal stages have been reformed so that the quantitative behavior of ERKN integrators is adapted to the oscillatory properties of the true solution. By the expansions for the errors of explicit ERKN integrators, we derive stiff order conditions up to order three and present the error bounds.

We show that the explicit ERKN integrator fulfilling stiff order p converges with order p, and *for an important particular case where M is a symmetric and positive semi-definite matrix, the error bound of $\|q_n - q(t_n)\|$ is independent of $\|M\|$ ($\|\cdot\|$ denotes the Euclidean norm)*. The stiff order conditions provided in the error analysis allow us to design new and efficient explicit ERKN integrators for multi-frequency oscillatory systems. We propose a novel explicit third order multi-frequency and multidimensional ERKN integrator with minimal dispersion error and dissipation error. Numerical experiments carried out show that our new explicit multi-frequency and multidimensional ERKN integrator is more efficient than various other existing effective methods in the scientific literature. We use the first problem to show that the methods perform well with nonsymmetric matrices. In particular, for the well-known Fermi–Pasta–Ulam problem, the numerical behavior of our new explicit ERKN integrator supports our theoretical analysis.

1. Introduction

Oscillatory problems are frequently encountered in many fields of applied sciences, such as applied mathematics, physics, astronomy, molecular dynamics and engineering. In particular, we often need to integrate systems of multi-frequency

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* Corresponding author.
E-mail addresses: wangbinmaths@gmail.com (B. Wang), xywu@nju.edu.cn (X. Wu), xiaj@math.purdue.edu (J. Xia).

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oscillatory second-order differential equations of the form

$$\begin{cases} q''(t) + Mq(t) = f\big(q(t)\big), & t \in [t_0, T], \\ q(t_0) = q_0, \qquad q'(t_0) = q'_0, \end{cases} \tag{1}$$

where M is a $d \times d$ positive semi-definite matrix implicitly containing the frequencies of the problem, and $q : [t_0, T] \to X$ is the solution of (1). Here $X = \mathcal{D}(q)$ and $\mathcal{D}(q)$ denotes the range of q. We note that the matrix M in (1) is not necessarily symmetric. A simple example of the oscillatory system (1) is

$$\begin{cases} q''(t) + \begin{pmatrix} 1 & 1 \\ 0 & 2 \end{pmatrix} q(t) = \mathbf{0}, & t \in [0, T], \\ q(0) = 1, \qquad q'(0) = 0, \end{cases}$$

where M is not symmetric. The Fermi–Pasta–Ulam problem [15,12] and the spatial semi-discretization of the wave equation with the method of lines are two classical examples of the form (1). Much research effort has been expended to find effective integrators for the oscillatory system (1). We refer the reader to [22] by Petzold et al., [2] by Cohen et al., and [33] by Wu et al., for surveys of existing mathematical and numerical approaches for oscillatory differential equations. For the case where M is a symmetric and positive semi-definite matrix, Hochbruck and Lubich develop Gautschi-type exponential integrators in [17]. The development of these methods can be traced back to [7] by Gautschi in 1961. Recently, some novel revised Runge–Kutta–Nyström (RKN) methods are also proposed for this case. See, e.g., [1,5,29,25,27,31,32,26] and the references therein. We refer the reader to [23,24,28,21] for some other revised RKN methods for (1) with the matrix M not necessarily symmetric. Very recently, Wu et al. [30] formulate a standard form of extended Runge–Kutta–Nyström (ERKN) methods for the multi-frequency oscillatory system (1). This form of ERKN integrators makes use of the special structure brought by the term Mq in (1), and does not require M in (1) to be symmetric. The corresponding order conditions for ERKN integrators are also given in [30]. On the other hand, it is very important to present the error analysis for ERKN integrators, which has not been discussed in [30]. In particular, it is interesting to show that the error bounds of an ERKN integrator are independent of $\|M\|$ if M is symmetric and positive semi-definite. Much progress has been made in the error analysis of numerical methods of ordinary differential equations (see, e.g., [16,13,20,18,19,3]). We note the results of error analysis related to numerical methods for the oscillatory system (1) with a symmetric and positive semi-definite matrix M, and refer the reader to [17,6,9–11]. In this paper, we present error bounds of explicit ERKN integrators for the multi-frequency oscillatory system (1) with a positive semi-definite matrix M which is not required to be symmetric.

We note that explicit ERKN integrators can deal with stiff problems, avoiding in this way the necessity of solving a system of nonlinear equations at each step. Consequently, we only consider the error analysis for explicit ERKN integrators in this paper. We present the error bounds of explicit ERKN integrators up to stiff order three. The resulting error bounds from the error analysis developed here provide new insight into ERKN integrators. Based on the stiff order conditions, we design a novel explicit ERKN integrator of order three with minimal dispersion error and dissipation error. The numerical results show that the new ERKN integrator is superior to some existing methods.

The rest of this paper is organized as follows. In Section 2, we summarize explicit ERKN integrators and present some basic results about the methods. Some preliminaries for the error analysis are given in Section 3, and the error bounds for explicit ERKN integrators are derived in Section 4. Section 5 is devoted to the development of a novel three-stage explicit multi-frequency and multidimensional ERKN integrator of order three with minimal dispersion error and dissipation error. In Section 6, we demonstrate the efficiency of the new method by the numerical experiments presented. We conclude the paper with some comments in the last section. Throughout the paper, the Euclidean norm for a matrix or a vector is denoted by $\|\cdot\|$.

2. Preliminaries for explicit ERKN integrators

In this section, we first reformulate explicit ERKN integrators for the system (1) and restate the corresponding order conditions. Then we analyze the stability and phase properties of explicit ERKN integrators.

In order to obtain asymptotic expansions for the exact solution of (1) similar to the G-functions used in [8] and the ϕ-functions given in [4], we introduce the following matrix-valued functions:

$$\phi_l(M) := \sum_{k=0}^{\infty} \frac{(-1)^k M^k}{(2k+l)!}, \quad l = 0, 1, \ldots. \tag{2}$$

Some interesting properties of these functions are established in the following proposition.

Proposition 2.1. *For $l = 0, 1, \ldots$, the ϕ-functions defined by (2) satisfy:*

(i) $\lim_{M \to \mathbf{0}} \phi_l(M) = \frac{1}{l!} I$, *where I is the identity matrix of the same order as M;*

(ii) *Next,*

$$\|\phi_l(M)\| \leqslant C, \tag{3}$$

where C is a constant depending on $\|M\|$ in general. In addition, for the particular and important case, where M is a symmetric and positive semi-definite matrix, C is independent of $\|M\|$;

(iii) *Also,*

$$\int_0^1 \frac{(1-\xi)\phi_1(a^2(1-\xi)^2M)\xi^j}{j!}\,d\xi = \phi_{j+2}(a^2M),$$
$$\int_0^1 \frac{\phi_0(a^2(1-\xi)^2M)\xi^j}{j!}\,d\xi = \phi_{j+1}(a^2M), \quad a \in \mathbb{R}. \tag{4}$$

Proof. It is observed that (i) is evident. We prove (ii) and (iii).

(ii): It is trivial to prove that the series $\sum_{k=0}^{\infty} \frac{x^k}{(2k+l)!}$ has the radius of convergence $r = +\infty$, and therefore

$$\|\phi_l(M)\| \leqslant \sum_{k=0}^{\infty} \frac{\|M\|^k}{(2k+l)!}.$$

Thus (3) is true.

In the important particular case where M is symmetric and positive semi-definite matrix, we have the decomposition of M as follows

$$M = P^T W^2 P = \Omega_0^2 \quad \text{with } \Omega_0 = P^T W P,$$

where P is an orthogonal matrix and $W = \mathrm{diag}(\lambda_i)$ with nonnegative diagonal entries which are the square roots of the eigenvalues of M. In this case,

$$\phi_l(M) = P^T \mathrm{diag}\big(\phi_l(\lambda_i^2)\big)P.$$

For all $x > 0$, $\phi_l(x)$ can be rewritten as $\phi_0(x) = \cos(\sqrt{x})$, $\phi_1(x) = \frac{\sin(\sqrt{x})}{\sqrt{x}}$, $\phi_{l+2}(x) = (\frac{1}{l!} - \phi_l(x))/x$, $l \geqslant 0$, which show that $\phi_l(x)$, $l = 0, 1, \ldots$ are uniformly bounded for $x > 0$. Since $\|P\| = 1$, we have the proof.

(iii): The first formula in (iii) can be shown as follows:

$$\int_0^1 \frac{(1-\xi)\phi_1(a^2(1-\xi)^2M)\xi^j}{j!}\,d\xi = \int_0^1 \frac{(1-\xi)\sum_{k=0}^{\infty}\frac{(-1)^k a^{2k}(1-\xi)^{2k}M^k}{(2k+1)!}\xi^j}{j!}\,d\xi$$
$$= \sum_{k=0}^{\infty}\int_0^1 \frac{(1-\xi)^{2k+1}\xi^j}{(2k+1)!\,j!}\,d\xi(-1)^k a^{2k}M^k = \sum_{k=0}^{\infty}\frac{(-1)^k a^{2k}M^k}{(2k+j+2)!} = \phi_{j+2}(a^2M).$$

Likewise, the second formula of (4) can be obtained in a straightforward way. □

It is clear that the definition in (2) depends directly on M and is applicable not only to symmetric matrices but also to nonsymmetric ones.

2.1. Explicit ERKN integrators and order conditions

For the exact solution of (1) and its derivative, we have the following variation-of-constants formula [30].

Theorem 2.2. *If $f : \mathbb{R}^d \to \mathbb{R}^d$ is continuous in (1), then for any real numbers t_0 and t, the solution of (1) and its derivative satisfy*

$$q(t) = \phi_0\big((t-t_0)^2M\big)q_0 + (t-t_0)\phi_1\big((t-t_0)^2M\big)q_0' + \int_{t_0}^{t}(t-\xi)\phi_1\big((t-\xi)^2M\big)\hat{f}(\xi)\,d\xi,$$
$$q'(t) = -(t-t_0)M\phi_1\big((t-t_0)^2M\big)q_0 + \phi_0\big((t-t_0)^2M\big)q_0' + \int_{t_0}^{t}\phi_0\big((t-\xi)^2M\big)\hat{f}(\xi)\,d\xi, \tag{5}$$

where $\hat{f}(\xi) = f(q(\xi))$.

Approximating the integrals in (5) by using some quadrature formulas leads to ERKN integrators for the system (1) in [30]. Here we only consider explicit ERKN schemes.

Definition 2.3. (See [30].) An s-stage explicit multi-frequency and multidimensional ERKN integrator for integrating the multi-frequency oscillatory system (1) is defined by

$$\begin{aligned} Y_{ni} &= \phi_0\big(c_i^2 V\big)q_n + hc_i\phi_1\big(c_i^2 V\big)q_n' + h^2\sum_{j=1}^{i-1}\bar{a}_{ij}(V)f(Y_{nj}), \quad i=1,2,\dots,s, \\ q_{n+1} &= \phi_0(V)q_n + h\phi_1(V)q_n' + h^2\sum_{i=1}^{s}\bar{b}_i(V)f(Y_{ni}), \\ q_{n+1}' &= -hM\phi_1(V)q_n + \phi_0(V)q_n' + h\sum_{i=1}^{s}b_i(V)f(Y_{ni}), \end{aligned} \tag{6}$$

where h is the stepsize, and $b_i(V)$, $\bar{b}_i(V)$ and $\bar{a}_{ij}(V)$, $i,j=1,2,\dots,s$, are matrix-valued functions of $V=h^2M$.

The coefficients of the scheme (6) can be arranged as a Butcher Tableau

$$\begin{array}{c|c} c & \bar{A}(V) \\ \hline & \bar{b}^T(V) \\ \hline & b^T(V) \end{array} = \begin{array}{c|cccc} c_1 & \mathbf{0}_{d\times d} & \mathbf{0}_{d\times d} & \cdots & \mathbf{0}_{d\times d} \\ c_2 & \bar{a}_{21}(V) & \mathbf{0}_{d\times d} & \cdots & \mathbf{0}_{d\times d} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & \bar{a}_{s1}(V) & \bar{a}_{s2}(V) & \cdots & \mathbf{0}_{d\times d} \\ \hline & \bar{b}_1(V) & \bar{b}_2(V) & \cdots & \bar{b}_s(V) \\ \hline & b_1(V) & b_2(V) & \cdots & b_s(V) \end{array} \tag{7}$$

Remark 2.4. It can be observed that the formula (5) does not depend on the decomposition of M, which is different from the one proposed by Hairer et al. (see [17,9,12,15]). Accordingly, our ERKN integrators avoid this kind of matrix decompositions. In this sense, (5) and (6) have broader applications in practice since the class of physical problems usually fall within the scope. Moreover, as $V \to \mathbf{0}_{d\times d}$, an ERKN integrator (6) reduces to a classical RKN method.

We define the order of ERKN integrators as follows.

Definition 2.5. An explicit ERKN integrator (6) for the system (1) has order r if for sufficiently smooth (1),

$$e_{n+1} := q_{n+1} - q(t_n+h) = \mathcal{O}\big(h^{r+1}\big), \qquad e_{n+1}' := q_{n+1}' - q'(t_n+h) = \mathcal{O}\big(h^{r+1}\big). \tag{8}$$

Here $q(t_n+h)$ and $q'(t_n+h)$ are the exact solution of (1) and the corresponding derivative at t_n+h, respectively, and q_{n+1} and q_{n+1}' are the numerical results obtained in one integration step under the local assumptions: $q_n=q(t_n)$ and $q_n'=q'(t_n)$.

Order conditions for ERKN integrators are presented in [30] and here we briefly restate the results in the following theorem.

Theorem 2.6. *An s-stage explicit ERKN integrator (6) is of order r if and only if*

$$\begin{aligned} \bar{b}^T(V)\Phi(\tau) &= \frac{\rho(\tau)!}{\gamma(\tau)}\phi_{\rho(\tau)+1}(V) + \mathcal{O}\big(h^{r-\rho(\tau)}\big), \quad \rho(\tau)=1,2,\dots,r-1, \\ b^T(V)\Phi(\tau) &= \frac{\rho(\tau)!}{\gamma(\tau)}\phi_{\rho(\tau)}(V) + \mathcal{O}\big(h^{r+1-\rho(\tau)}\big), \quad \rho(\tau)=1,2,\dots,r, \end{aligned}$$

where τ is an extended Nyström tree associated with an elementary differential $\mathcal{F}(\tau)(q_n,q_n')$ of the function $f(q)$ at q_n.

The set of extended Nyström trees $\mathbb{T}$, the functions $\rho(\tau)$, the *order* of τ, $\alpha(\tau)$, the *number of possible monotonic labellings* of τ, and $\gamma(\tau)$, the *signed density* of τ, are well defined in [34]. The elementary differential $\mathcal{F}$ and the vector $\Phi(\tau)=(\Phi_i(\tau))_{i=1}^{s}$ of elementary weights for the internal stages can also be found in [34].

2.2. Stability and phase properties

It is known that when applied a numerical method to solving oscillatory differential equations, it usually produces some dispersion and/or dissipation, even if the method may be of high algebraic orders.

We now turn to the stability and phase properties of explicit ERKN integrators. Following [23], we use a second-order homogeneous linear test model of the form

$$q''(t) + \omega^2 q(t) = -\epsilon q(t), \quad \omega^2 + \epsilon > 0, \tag{9}$$

where ω represents an estimation of the dominant frequency λ and $\epsilon = \lambda^2 - \omega^2$ is the error of the estimation. Applying an explicit ERKN integrator (6) to the test equation (9) yields

$$\begin{aligned} &Y = \phi_0\big(c^2V\big)q_n + \big(c \cdot \phi_1\big(c^2V\big)h\big)q_n' - z\bar{A}(V)Y, \quad z = \epsilon h^2, \quad V = h^2\omega^2, \\ &q_{n+1} = \phi_0(V)q_n + \phi_1(V)hq_n' - z\bar{b}^T(V)Y, \\ &hq_{n+1}' = -V\phi_1(V)q_n + \phi_0(V)hq_n' - zb^T(V)Y. \end{aligned} \tag{10}$$

Thus,

$$\begin{pmatrix} q_{n+1} \\ hq_{n+1}' \end{pmatrix} = S(V,z)\begin{pmatrix} q_n \\ hq_n' \end{pmatrix},$$

where the stability matrix $S(V,z)$ is determined by

$$S(V,z) = \begin{pmatrix} \phi_0(V) - z\bar{b}^T(V)N^{-1}\phi_0(c^2V) & \phi_1(V) - z\bar{b}^T(V)N^{-1}(c \cdot \phi_1(c^2V)) \\ -V\phi_1(V) - zb^T(V)N^{-1}\phi_0(c^2V) & \phi_0(V) - zb^T(V)N^{-1}(c \cdot \phi_1(c^2V)) \end{pmatrix},$$

with $N = I + z\bar{A}(V)$.

The stability of an explicit ERKN integrator is characterized by the spectral radius $\rho(S(V,z))$. We use the two-dimensional region (V,z)-plane to express the stability of an explicit ERKN integrator:

- $R_s = \{(V,z) \mid V > 0 \text{ and } \rho(S) < 1\}$ is called the *stability region* of an explicit ERKN integrator;
- $R_p = \{(V,z) \mid V > 0,\ \rho(S) = 1 \text{ and } \mathrm{tr}(S)^2 < 4\det(S)\}$ is called the *periodicity region* of an explicit ERKN integrator;
- If $R_s = (0,+\infty) \times (-\infty,+\infty)$, the explicit ERKN integrator is said to be *A-stable*;
- If $R_p = (0,+\infty) \times (-\infty,+\infty)$, the explicit ERKN integrator is said to be *P-stable*.

The dispersion error and the dissipation error can be defined in a way similar to those described in [23].

Definition 2.7. Let $H := h\lambda = \sqrt{V+z}$ and

$$\phi := H - \arccos\left(\frac{\mathrm{tr}(S(V,z))}{2\sqrt{\det(S(V,z))}}\right), \qquad d := 1 - \sqrt{\det\big(S(V,z)\big)},$$

where $z = \frac{\epsilon}{\omega^2+\epsilon}H^2$, $V = \frac{\omega^2}{\omega^2+\epsilon}H^2$. Then the Taylor expansions of ϕ and d in H (denoted by $\phi(H)$ and $d(H)$) are called the dispersion error and the dissipation error of the explicit ERKN integrator, respectively. Thus, a method is said to be dispersive of order r if $\phi(H) = \mathcal{O}(H^{r+1})$, and is said to be dissipative of order s if $d(H) = \mathcal{O}(H^{s+1})$. If $\phi(H) = 0$ and $d(H) = 0$, then the method is said to be zero dispersive and zero dissipative, respectively.

3. Preliminaries of error analysis

In the following analysis, we restrict ourselves to the case of s-stage explicit ERKN integrators of order p with $s \leqslant 3$ and $p \leqslant 3$.

3.1. Three elementary assumptions and a Gronwall's lemma

Throughout the paper we use the following three elementary assumptions for the error analysis of explicit ERKN integrators.

Assumption 3.1. We suppose that (1) possesses a uniformly bounded and sufficiently smooth solution $q : [t_0, T] \to X$ with derivatives in X, and that $f(q) : X \to S$ in (1) is sufficiently often Frèchet differentiable in a strip (see [18,19]) along the exact solution of (1). All occurring derivatives of $f(q)$ are supposed to be uniformly bounded.

Assumption 3.2. The coefficients of an s-stage explicit ERKN integrator (6) satisfy the following assumptions:

$$\sum_{j=1}^{i-1} \bar{a}_{ij}(V) = c_i^2 \phi_2\big(c_i^2 V\big), \quad i = 1, 2, \ldots, s. \tag{11}$$

Note that (11) implies $c_1 = 0$.

Assumption 3.3. The coefficients $b_i(V)$, $\bar{b}_i(V)$ and $\bar{a}_{ij}(V)$, $i, j = 1, 2, \ldots, s$, of an s-stage explicit ERKN integrator (6) are bounded for any matrix V and uniformly bounded for symmetric and positive semi-definite ones.

In the following analysis, we will use a discrete Gronwall's lemma (Lemma 2.4 in [16]). Here, we represent the lemma as follows.

Lemma 3.4. *Let α, ϕ, ψ, and χ be nonnegative functions defined for $t = n\Delta t$, $n = 0, 1, \ldots, M$, and assume χ is nondecreasing. If*

$$\phi_k + \psi_k \leqslant \chi_k + \Delta t \sum_{n=1}^{k-1} \alpha_n \phi_n, \quad k = 1, 2, \ldots, M,$$

and if there is a positive constant $\hat{c}$ such that $\Delta t \sum_{n=1}^{k-1} \alpha_n \leqslant \hat{c}$, then

$$\phi_k + \psi_k \leqslant \chi_k e^{\hat{c} k \Delta t}, \quad k = 1, 2, \ldots, M,$$

where the subscript indices k and n denote the values of functions at $t_k = k\Delta t$ and $t_n = n\Delta t$, respectively.

3.2. Discrepancies

As for the preliminaries, we first work on the discrepancy estimation for explicit ERKN integrators.
Inserting the exact solution of (1) into the numerical scheme (6) gives

$$\begin{aligned}
&q(t_n + c_i h) = \phi_0\big(c_i^2 V\big) q(t_n) + h c_i \phi_1\big(c_i^2 V\big) q'(t_n) + h^2 \sum_{j=1}^{i-1} \bar{a}_{ij}(V) \hat{f}(t_n + c_j h) + \Delta_{ni}, \quad i = 1, 2, \ldots, s, \\
&q(t_n + h) = \phi_0(V) q(t_n) + h \phi_1(V) q'(t_n) + h^2 \sum_{i=1}^{s} \bar{b}_i(V) \hat{f}(t_n + c_i h) + \delta_{n+1}, \\
&q'(t_n + h) = -hM \phi_1(V) q(t_n) + \phi_0(V) q'(t_n) + h \sum_{i=1}^{s} b_i(V) \hat{f}(t_n + c_i h) + \delta'_{n+1},
\end{aligned} \tag{12}$$

where Δ_{ni}, δ_{n+1} and δ'_{n+1} are the discrepancies and $\hat{f}(t) = f(q(t))$. The following Lemma gives an estimation of the discrepancies.

Lemma 3.5. *Under Assumptions 3.1, 3.2 and 3.3, if the stiff order conditions (Table 1) of explicit ERKN integrators are satisfied up to order p ($p \leqslant 3$), then*

$$\begin{aligned}
&\|\Delta_{n1}\| = 0, \\
&\|\Delta_{ni}\| \leqslant C_1 h^3, \quad i = 2, 3, \\
&\|\delta_{n+1}\| \leqslant C_2 h^{p+1}, \\
&\|\delta'_{n+1}\| \leqslant C_3 h^{p+1}.
\end{aligned} \tag{13}$$

Here the constants C_1, C_2 and C_3 depend on $\|M\|$ but are independent of h and n. In addition, in the important particular case where M is symmetric and positive semi-definite, they are all independent of $\|M\|$.

Proof. Expressing $q(t_n + c_i h)$ in (12) by the formula (5) yields

$$q(t_n + c_i h) = \phi_0\big(c_i^2 V\big) q(t_n) + h c_i \phi_1\big(c_i^2 V\big) q'(t_n) + h^2 \int_0^{c_i} (c_i - z) \phi_1\big((c_i - z)^2 V\big) \hat{f}(t_n + hz)\, dz. \tag{14}$$

Table 1
Stiff order conditions for explicit ERKN integrators

Stiff order conditions	Order
$\sum_{i=1}^{s} b_i(V) = \phi_1(V)$	1
$\sum_{i=1}^{s} b_i(V)c_i = \phi_2(V)$	2
$\sum_{i=1}^{s} \bar{b}_i(V) = \phi_2(V)$	2
$\sum_{j=1}^{i-1} \bar{a}_{ij}(V) = c_i^2\phi_2(c_i^2 V),\ \ i = 1, 2, \ldots, s$	3
$\sum_{i=1}^{s} b_i(V)c_i^2 = 2\phi_3(V)$	3
$\sum_{i=1}^{s} \bar{b}_i(V)c_i = \phi_3(V)$	3

Comparing (14) with the first formula in (12), we obtain

$$\Delta_{ni} = h^2 \int_0^{c_i} (c_i - z)\phi_1\big((c_i - z)^2 V\big)\hat{f}(t_n + hz)\,dz - h^2 \sum_{j=1}^{i-1} \bar{a}_{ij}(V)\hat{f}(t_n + c_j h).$$

Expressing $\hat{f}(t_n + hz)$ of the above formula by the Taylor series expansion yields

$$\begin{aligned}
\Delta_{ni} &= h^2 \int_0^{c_i} (c_i - z)\phi_1\big((c_i - z)^2 V\big) \sum_{j=0}^{\infty} \frac{h^j z^j}{j!} \hat{f}^{(j)}(t_n)\,dz - h^2 \sum_{k=1}^{i-1} \bar{a}_{ik}(V) \sum_{j=0}^{\infty} \frac{c_k^j h^j}{j!} \hat{f}^{(j)}(t_n) \\
&= \sum_{j=0}^{\infty} h^{j+2} c_i^{j+2} \int_0^1 \frac{(1-\xi)\phi_1(c_i^2(1-\xi)^2 V)\xi^j}{j!}\,d\xi\, \hat{f}^{(j)}(t_n) - h^2 \sum_{k=1}^{i-1} \bar{a}_{ik}(V) \sum_{j=0}^{\infty} \frac{c_k^j h^j}{j!} \hat{f}^{(j)}(t_n).
\end{aligned}$$

By the third property of Proposition 2.1, we have

$$\begin{aligned}
\Delta_{ni} &= \sum_{j=0}^{\infty} h^{j+2} c_i^{j+2} \phi_{j+2}\big(c_i^2 V\big)\hat{f}^{(j)}(t_n) - h^2 \sum_{k=1}^{i-1} \bar{a}_{ik}(V) \sum_{j=0}^{\infty} \frac{c_k^j h^j}{j!} \hat{f}^{(j)}(t_n) \\
&= \sum_{j=0}^{\infty} h^{j+2} \left[c_i^{j+2} \phi_{j+2}\big(c_i^2 V\big) - \sum_{k=1}^{i-1} \bar{a}_{ik}(V) \frac{c_k^j}{j!} \right] \hat{f}^{(j)}(t_n).
\end{aligned}$$

It follows from Assumptions 3.1 and 3.2 that

$$\|\Delta_{n1}\| = 0, \qquad \|\Delta_{ni}\| \leqslant C_1 h^3, \quad i = 2, 3.$$

Similarly, for δ_{n+1}, we have

$$\begin{aligned}
\delta_{n+1} &= h^2 \int_0^1 (1 - z)\phi_1\big((1 - z)^2 V\big)\hat{f}(t_n + hz)\,dz - h^2 \sum_{k=1}^{s} \bar{b}_k(V)\hat{f}(t_n + c_k h) \\
&= h^2 \int_0^1 (1 - z)\phi_1\big((1 - z)^2 V\big) \sum_{j=0}^{\infty} \frac{h^j z^j}{j!} \hat{f}^{(j)}(t_n)\,dz - h^2 \sum_{k=1}^{s} \bar{b}_k(V) \sum_{j=0}^{\infty} \frac{c_k^j h^j}{j!} \hat{f}^{(j)}(t_n) \\
&= \sum_{j=0}^{\infty} h^{j+2} \int_0^1 \frac{(1-z)\phi_1((1-z)^2 V) z^j}{j!}\,dz \hat{f}^{(j)}(t_n) - h^2 \sum_{k=1}^{i-1} \bar{b}_k(V) \sum_{j=0}^{\infty} \frac{c_k^j h^j}{j!} \hat{f}^{(j)}(t_n) \\
&= \sum_{j=0}^{\infty} h^{j+2} \phi_{j+2}(V)\hat{f}^{(j)}(t_n) - h^2 \sum_{k=1}^{i-1} \bar{b}_k(V) \sum_{j=0}^{\infty} \frac{c_k^j h^j}{j!} \hat{f}^{(j)}(t_n) \\
&= \sum_{j=0}^{\infty} h^{j+2} \left[\phi_{j+2}(V) - \sum_{k=1}^{i-1} \bar{b}_k(V) \frac{c_k^j}{j!} \right] \hat{f}^{(j)}(t_n).
\end{aligned}$$

The third formula in (13) follows immediately from the stiff order conditions for ERKN integrators of order p (Table 1).

Likewise, we get

$$\delta'_{n+1} = \sum_{j=0}^{\infty} h^{j+1}\left[\phi_{j+1}(V) - \sum_{k=1}^{s} b_k(V)\frac{c_k^j}{j!}\right]\hat{f}^{(j)}(t_n),$$

and the fourth formula in (13) holds. □

Remark 3.6. All conditions encountered so far in the above proof are collected in Table 1. It is easy to check that these conditions can yield the corresponding order conditions (Theorem 2.6). However, these conditions are different from those given in Theorem 2.6, since they use the assumption (11) plus some order conditions (Theorem 2.6) with the terms $\mathcal{O}(h^{r-\rho(\tau)})$ and $\mathcal{O}(h^{r+1-\rho(\tau)})$ ignored in these order conditions. The conditions shown in Table 1 are considered as stiff order conditions (following [18,19]). We restrict ourselves to the explicit ERKN integrators that fulfill the stiff order conditions up to order p ($p \leqslant 3$) in the remaining parts of this paper. For the important particular case where M is symmetric and positive semi-definite, it is important to observe that the constants C_1, C_2, and C_3 are all independent of $\|M\|$ for the reason that $\phi_l(V)$, $b_i(V)$, $\bar{b}_i(V)$, and $\bar{a}_{ij}(V)$ ($l = 0, 1, \ldots$ and $i, j = 1, 2, \ldots, s$) are all uniformly bounded.

4. Error bounds

Let e_n denote the difference between the numerical and exact solutions at t_n, E_{ni} the difference at $t_n + c_i h$, and e'_n the difference between the numerical and exact derivatives at t_n, namely,

$$e_n = q_n - q(t_n), \qquad E_{ni} = Y_{ni} - q(t_n + c_i h), \qquad e'_n = q'_n - q'(t_n). \tag{15}$$

Subtracting (12) from (6) gives the error recursions

$$\begin{aligned}
E_{ni} &= \phi_0\big(c_i^2 V\big)e_n + hc_i\phi_1\big(c_i^2 V\big)e'_n + h^2\sum_{j=1}^{i-1}\bar{a}_{ij}(V)\big[f(Y_{nj}) - \hat{f}(t_n + c_j h)\big] - \Delta_{ni}, \quad i = 1, 2, \ldots, s,\\
e_{n+1} &= \phi_0(V)e_n + h\phi_1(V)e'_n + h^2\sum_{i=1}^{s}\bar{b}_i(V)\big[f(Y_{ni}) - \hat{f}(t_n + c_i h)\big] - \delta_{n+1},\\
e'_{n+1} &= -hM\phi_1(V)e_n + \phi_0(V)e'_n + h\sum_{i=1}^{s} b_i(V)\big[f(Y_{ni}) - \hat{f}(t_n + c_i h)\big] - \delta'_{n+1}.
\end{aligned} \tag{16}$$

In what follows we propose two lemmas from which we present the main result of the analysis in this paper.

Lemma 4.1. *Under Assumptions 3.1, 3.2 and 3.3, if the errors e_n and e'_n remain in a neighborhood of 0, then*

$$\begin{aligned}
&\big\|f(Y_{ni}) - \hat{f}(t_n + c_i h)\big\| \leqslant C_4\big(\|E_{ni}\| + \|E_{ni}\|^2\big), \quad i = 1, 2, 3,\\
&\|E_{ni}\| \leqslant C_5\big(\|e_n\| + h\big\|e'_n\big\| + h^3\big), \quad i = 1, 2, 3,
\end{aligned} \tag{17}$$

where the constants C_4 and C_5 depend on $\|M\|$ but are independent of h and n. In the important particular case where M is a symmetric and positive semi-definite matrix, C_4 and C_5 are both independent of $\|M\|$.

Proof. The Taylor series expansion of $\hat{f}(t_n + c_i h)$ yields

$$\begin{aligned}
f(Y_{ni}) - \hat{f}(t_n + c_i h) = f(Y_{ni}) - f\big(q(t_n + c_i h)\big) &= \frac{\partial f}{\partial q}\big(q(t_n + c_i h)\big)E_{ni}\\
&\quad + \int_0^1 (1-\tau)\frac{\partial^2 f}{\partial q^2}\big(q(t_n + c_i h) + \tau E_{ni}\big)(E_{ni}, E_{ni})\,d\tau.
\end{aligned}$$

This formula proves immediately the first inequality of (17) by Assumption 3.1.

By setting $i = 1$ in the first formula of (16), it is trivial to verify that

$$\|E_{n1}\| = \|e_n\|. \tag{18}$$

It follows from the first formula of (16) and the first formula of (17) that

$$\|E_{ni}\| \leqslant C_6\|e_n\| + C_7 h\big\|e'_n\big\| + C_8 h^2\sum_{j=1}^{i-1}\big(\|E_{nj}\| + \|E_{nj}\|^2\big) + \|\Delta_{ni}\|, \quad i = 2, 3. \tag{19}$$

By Lemma 3.5, we obtain

$$\|E_{ni}\| \leqslant C_6\|e_n\| + C_7h\|e'_n\| + C_8h^2\sum_{j=1}^{i-1}\left(\|E_{nj}\| + \|E_{nj}\|^2\right) + C_1h^3. \tag{20}$$

Thus the following result holds as long as the error e_n remains in a neighborhood of 0:

$$\begin{aligned}\|E_{n2}\| &\leqslant C_6\|e_n\| + C_7h\|e'_n\| + C_8h^2\left(\|E_{n1}\| + \|E_{n1}\|^2\right) + C_1h^3\\ &= C_6\|e_n\| + C_7h\|e'_n\| + C_8h^2\left(\|e_n\| + \|e_n\|^2\right) + C_1h^3\\ &= \left(C_6 + C_8h^2 + +C_8h^2\|e_n\|\right)\|e_n\| + C_7h\|e'_n\| + C_1h^3\\ &\leqslant \widetilde{C}_2\left(\|e_n\| + h\|e'_n\| + h^3\right).\end{aligned}$$

In similar way, we obtain

$$\|E_{n3}\| \leqslant \widetilde{C}_3\left(\|e_n\| + h\|e'_n\| + h^3\right).$$

Letting $C_5 = \max(1, \widetilde{C}_2, \widetilde{C}_3)$ yields immediately

$$\|E_{ni}\| \leqslant C_5\left(\|e_n\| + h\|e'_n\| + h^3\right), \quad i = 1, 2, 3. \qquad \square$$

Lemma 4.2. *Under Assumptions 3.1, 3.2 and 3.3, consider an s-stage ($s \leqslant 3$) explicit ERKN integrator (6) that fulfills the stiff order conditions up to order p ($p \leqslant 3$) for the system (1). Then the numerical solution and its derivative satisfy the following inequalities uniformly on $0 \leqslant nh \leqslant T - t_0$:*

$$\begin{aligned}\|e_n\| &\leqslant \bar{C}h^p + \bar{C}\sum_{k=0}^{n-1}\left(h^2 + h^3\right)\left\{\|e'_k\| + h\|e'_k\|^2\right\},\\ \|e'_n\| &\leqslant \widetilde{C}h^p + \widetilde{C}\sum_{k=0}^{n-1}\left(h + h^2\right)\left\{\|e_k\| + h^3\|e_k\| + \|e_k\|^2\right\},\end{aligned} \tag{21}$$

where $\bar{C}$ and $\widetilde{C}$ are constants depending on T and $\|M\|$ but independent of h and n. In addition, in the important particular case where M is symmetric and positive semi-definite, $\bar{C}$ is independent of $\|M\|$.

Proof. From (16), we obtain the error recursion

$$\begin{pmatrix} e_{n+1}\\ e'_{n+1}\end{pmatrix} = Q\begin{pmatrix} e_n\\ e'_n\end{pmatrix} + \begin{pmatrix} h^2\sum_{i=1}^s \bar{b}_i(V)[f(Y_{ni}) - \hat{f}(t_n + c_ih)] - \delta_{n+1}\\ h\sum_{i=1}^s b_i(V)[f(Y_{ni}) - \hat{f}(t_n + c_ih)] - \delta'_{n+1}\end{pmatrix}.$$

Solving this recursion yields

$$\begin{pmatrix} e_n\\ e'_n\end{pmatrix} = \sum_{k=0}^{n-1} Q^{n-k-1}\begin{pmatrix} h^2\sum_{i=1}^s \bar{b}_i(V)[f(Y_{ki}) - \hat{f}(t_k + c_ih)] - \delta_{k+1}\\ h\sum_{i=1}^s b_i(V)[f(Y_{ki}) - \hat{f}(t_k + c_ih)] - \delta'_{k+1}\end{pmatrix},$$

where $e_0 = \mathbf{0}$, $e'_0 = \mathbf{0}$ are used, and

$$Q = \begin{pmatrix} \phi_0(V) & h\phi_1(V)\\ -hM\phi_1(V) & \phi_0(V)\end{pmatrix}, \qquad Q^m = \begin{pmatrix} \phi_0(m^2V) & mh\phi_1(m^2V)\\ -mhM\phi_1(m^2V) & \phi_0(m^2V)\end{pmatrix}.$$

By $\|m^2V\| \leqslant T^2\|M\|$ and Proposition 2.1,

$$\left\|\phi_0\left(m^2V\right)\right\| \leqslant C \quad \text{and} \quad \left\|mh\phi_1\left(m^2V\right)\right\| \leqslant T\left\|\phi_1\left(m^2V\right)\right\| \leqslant C. \tag{22}$$

Thus

$$\begin{aligned}\|e_n\| &\leqslant \sum_{k=0}^{n-1}\left\{C\left(h^2\sum_{i=1}^s\left\|f(Y_{ki}) - \hat{f}(t_k + c_ih)\right\| + \|\delta_{k+1}\|\right) + C\left(h\sum_{i=1}^s\left\|f(Y_{ki}) - \hat{f}(t_k + c_ih)\right\| + \left\|\delta'_{k+1}\right\|\right)\right\}\\ &\leqslant C\sum_{k=0}^{n-1}\left\{\left(h^2 + h\right)\sum_{i=1}^s\left\|f(Y_{ki}) - \hat{f}(t_k + c_ih)\right\| + \|\delta_{k+1}\| + \left\|\delta'_{k+1}\right\|\right\}.\end{aligned}$$

A direct application of the equations in Lemma 4.1 gives

$$\|e_n\| \leqslant C\sum_{k=0}^{n-1}\left\{(h^2+h)\sum_{i=1}^{s}C_4\left[C_5\left(\|e_k\|+h\left\|e'_k\right\|+h^3\right)+\left(C_5\left(\|e_k\|+h\left\|e'_k\right\|+h^3\right)\right)^2\right]+\|\delta_{k+1}\|+\left\|\delta'_{k+1}\right\|\right\}.$$

It follows from Lemma 3.5 that

$$\begin{aligned}\|e_n\| &\leqslant C\sum_{k=0}^{n-1}\left\{(h^2+h)\left[C_6\left(\|e_k\|+h\left\|e'_k\right\|+h^3\right)+\left(C_6\left(\|e_k\|+h\left\|e'_k\right\|+h^3\right)\right)^2\right]+C_2h^{p+1}+C_3h^{p+1}\right\}\\ &\leqslant C\sum_{k=0}^{n-1}\left\{(h^2+h)\left[C_6h\left\|e'_k\right\|+C_6^2h^2\left\|e'_k\right\|^2\right]+\check{C}h^{p+1}\right\}\\ &\quad+h\sum_{k=0}^{n-1}C(h+1)\left[C_6+C_6^2\|e_k\|+2C_6h\left\|e'_k\right\|+2C_6h^3\right]\|e_k\|,\end{aligned} \tag{23}$$

where $\check{C}$ is a constant which can be chosen such that the above formula is true. Considering Lemma 3.4, we set

$$\begin{aligned}&\phi_n=\|e_n\|,\qquad \psi_n\equiv 0,\\ &\chi_n=C\sum_{k=0}^{n-1}\left\{(h^2+h)\left[C_6h\left\|e'_k\right\|+C_6^2h^2\left\|e'_k\right\|^2\right]+\check{C}h^{p+1}\right\},\\ &\alpha_k=C(h+1)\left[C_6+C_6^2\|e_k\|+2C_6h\left\|e'_k\right\|+2C_6h^3\right].\end{aligned}$$

Therefore, as long as the errors e_n and e'_n remain in a neighborhood of 0, the following result holds:

$$\begin{aligned}h\sum_{k=0}^{n-1}\alpha_k &= h\sum_{k=0}^{n-1}C(h+1)\left[C_6+C_6^2\|e_k\|+2C_6h\left\|e'_k\right\|+2C_6h^3\right]\\ &\leqslant Cnh(h+1)\left[C_6+C_6^2C_7+2C_6hC_7+2C_6h^3\right]\\ &\leqslant CT(h+1)\left[C_6+C_6^2C_7+2C_6hC_7+2C_6h^3\right]\leqslant C_8.\end{aligned}$$

The application of the discrete Gronwall lemma, Lemma 3.4, to (23) gives

$$\|e_n\|\leqslant\widehat{C}\sum_{k=0}^{n-1}h^{p+1}+\widehat{C}\sum_{k=0}^{n-1}(h^2+h)\left\{h\left\|e'_k\right\|+h^2\left\|e'_k\right\|^2\right\}\leqslant\bar{C}h^p+\bar{C}\sum_{k=0}^{n-1}(h^2+h^3)\left\{\left\|e'_k\right\|+h\left\|e'_k\right\|^2\right\}, \tag{24}$$

where $\bar{C}$ is a constant depending on T and $\|M\|$ but independent of h and n. In addition, for the important particular case where M is symmetric and positive semi-definite, $\bar{C}$ is independent of $\|M\|$.

Likewise, from

$$\left\|\phi_0\left(m^2V\right)\right\|\leqslant C\quad\text{and}\quad\left\|-mhM\phi_1\left(m^2V\right)\right\|\leqslant C\|M\|, \tag{25}$$

it follows that

$$\left\|e'_n\right\|\leqslant\widetilde{C}h^p+\widetilde{C}\sum_{k=0}^{n-1}(h+h^2)\left\{\|e_k\|+h^3\|e_k\|+\|e_k\|^2\right\}. \tag{26}$$

The constant $\widetilde{C}$ depends on $\|M\|$ and T but is independent of h and n. □

Remark 4.3. It is noted that by Proposition 2.1, for the important particular case where M is symmetric and positive semi-definite, the constant C of inequality (22) is independent of $\|M\|$. Moreover, in this case, the constants C_i, $i=1,2,\ldots,5$, in formulas (13) and (17) are all independent of $\|M\|$. Therefore, when M is symmetric and positive semi-definite, $\bar{C}$ in the above lemma is independent of $\|M\|$, and the fact stated above also results in the conclusion that the error bound of $\|e_n\|$ given in the following theorem is independent of $\|M\|$.

We are now ready to present the main result of this paper.

Theorem 4.4. *Under the conditions of Lemma 4.2, the explicit ERKN integrator (6) converges for $0 \leqslant nh \leqslant T - t_0$. In particular, the numerical solution and its derivative satisfy the following error bounds*

$$\begin{aligned} \|e_n\| &\leqslant \widehat{C}_1 h^p, \\ \|e'_n\| &\leqslant \widehat{C}_2 h^p, \end{aligned} \tag{27}$$

where the constant $\widehat{C}_1 = \bar{C} + 1$ depends on T and $\|M\|$ but is independent of h and n. The constant $\widehat{C}_2 = \widetilde{C} + \widetilde{C}T\widehat{C}_1 + 1$ depends on $\|M\|$ and T, but is independent of h and n. In addition, in the important particular case where M is symmetric and positive semi-definite, $\widehat{C}_1$ is independent of $\|M\|$.

Proof. By $e_0 = \mathbf{0}$, $e'_0 = \mathbf{0}$, and (21), it is easy to verify that $\|e_1\|$ and $\|e'_1\|$ satisfy (27). Then we prove this theorem by induction. Suppose the inequalities (27) hold for k ($k \leqslant n$), we prove the result for $n+1$. By the formula (21),

$$\|e_{n+1}\| \leqslant \bar{C}h^p + \bar{C}\sum_{k=0}^{n}(h^2 + h^3)\left[\|e'_k\| + h\|e'_k\|^2\right].$$

By the assumption that the inequalities (27) hold for $i \leqslant n$, we obtain

$$\begin{aligned} \|e_{n+1}\| &\leqslant \bar{C}h^p + \bar{C}\sum_{k=0}^{n}(h^2 + h^3)\left[\widehat{C}_2 h^p + h\left(\widehat{C}_2 h^p\right)^2\right] \\ &\leqslant \bar{C}h^p + \bar{C}(n+1)\left(h^2 + h^3\right)\left[\widehat{C}_2 h^p + h\left(\widehat{C}_2 h^p\right)^2\right] \\ &\leqslant \bar{C}h^p + \bar{C}T\left(h + h^2\right)\left[\widehat{C}_2 h^p + h\left(\widehat{C}_2 h^p\right)^2\right] \\ &\leqslant (\bar{C}+1)h^p. \end{aligned}$$

This shows that the first inequality of (27) holds for $n+1$. Note that for the discussion of convergence, we always mean to consider $h \to 0$. Therefore, we use the assumption of $h\Upsilon \leqslant 1$ in the above formula, where Υ can be a large positive but finite number. In a similar way, we obtain

$$\begin{aligned} \|e'_{n+1}\| &\leqslant \widetilde{C}h^p + \widetilde{C}\sum_{k=0}^{n}\left(h + h^2\right)\left\{\|e_k\| + h^3\|e_k\| + \|e_k\|^2\right\} \\ &\leqslant \widetilde{C}h^p + \widetilde{C}\sum_{k=0}^{n}\left(h + h^2\right)\left\{\widehat{C}_1 h^p + h^3\widehat{C}_1 h^p + \left(\widehat{C}_1 h^p\right)^2\right\} \\ &\leqslant \widetilde{C}h^p + \widetilde{C}T(1+h)\left\{\widehat{C}_1 h^p + h^3\widehat{C}_1 h^p + \left(\widehat{C}_1 h^p\right)^2\right\} \\ &\leqslant \left(\widetilde{C} + \widetilde{C}T\widehat{C}_1 + 1\right)h^p. \end{aligned}$$

This formula yields the second inequality of (27) for $n+1$. Hence, we have proved the theorem. $\square$

Remark 4.5. The key point to be noted here is that the error analysis of the explicit ERKN integrators derived in this paper is not dependent on the matrix decomposition of M, unlike the error analysis of Gautschi-type exponential integrators (see [9–11,15]). Our error analysis for ERKN integrators is applicable to not only symmetric M but also nonsymmetric M. Our error analysis therefore has wider applications in general.

Remark 4.6. It has been pointed out in Remark 4.3 that, for the important particular case where M is symmetric and positive semi-definite, $\bar{C}$ in Lemma 4.2 is independent of $\|M\|$. By the formula $\widehat{C}_1 = \bar{C} + 1$ given in Theorem 4.4, it is clear that for the symmetric matrix, the error bound of $\|e_n\|$ does not depend on $\|M\|$. In fact, in highly oscillatory problems, $\|M\|$ can be arbitrarily large. Moreover, Table 1 presents the stiff order conditions up to order three and from which, a more effective explicit ERKN integrator is designed in the next section to solve (1) numerically. Therefore, the error analysis for ERKN integrators is not only a significant theoretical result but also a contribution to constructing numerical methods for solving (1) in practical applications.

5. An explicit third order multi-frequency and multidimensional ERKN integrator with minimal dispersion error and dissipation error

In this section, we propose an explicit three-stage multi-frequency and multidimensional ERKN integrator of order three with minimal dispersion error and dissipation error. First, the scheme (6) of a three-stage explicit ERKN integrator can be denoted by the Butcher tableau

$$\begin{array}{c|ccc} c_1 & \mathbf{0}_{d\times d} & \mathbf{0}_{d\times d} & \mathbf{0}_{d\times d} \\ c_2 & \bar{a}_{21}(V) & \mathbf{0}_{d\times d} & \mathbf{0}_{d\times d} \\ c_3 & \bar{a}_{31}(V) & \bar{a}_{32}(V) & \mathbf{0}_{d\times d} \\ \hline & \bar{b}_1(V) & \bar{b}_2(V) & \bar{b}_3(V) \\ \hline & b_1(V) & b_2(V) & b_3(V) \end{array}$$

From the stiff order conditions of Table 1, three-stage explicit ERKN integrators of order three are given by:

$$\begin{aligned} &b_1(V)+b_2(V)+b_3(V)=\phi_1(V), \\ &b_1(V)c_1+b_2(V)c_2+b_3(V)c_3=\phi_2(V), \\ &b_1(V)c_1^2+b_2(V)c_2^2+b_3(V)c_3^2=2\phi_3(V), \\ &c_1=0, \qquad \bar{a}_{21}(V)=c_2^2\phi_2\big(c_2^2V\big), \\ &\bar{a}_{31}(V)+\bar{a}_{32}(V)=c_3^2\phi_2\big(c_3^2V\big), \\ &\bar{b}_1(V)+\bar{b}_2(V)+\bar{b}_3(V)=\phi_2(V), \\ &\bar{b}_1(V)c_1+\bar{b}_2(V)c_2+\bar{b}_3(V)c_3=\phi_3(V). \end{aligned} \tag{28}$$

Since these conditions are not sufficient to determine the coefficients of a three-stage explicit ERKN integrator, we also consider two more conditions (obtained by modifying the two equations in Theorem 2.6):

$$\begin{aligned} &\bar{b}_1(V)c_1^2+\bar{b}_2(V)c_2^2+\bar{b}_3(V)c_3^2=2\phi_4(V), \\ &b_3(V)\big(\bar{a}_{31}(V)c_1+\bar{a}_{32}(V)c_2\big)=\phi_4(V). \end{aligned} \tag{29}$$

Choosing c_2, c_3 as parameters and solving all the equations in (28) and (29) give

$$\begin{aligned} &b_1(V)=\frac{c_2c_3\phi_1(V)-(c_2+c_3)\phi_2(V)+2\phi_3(V)}{c_2c_3}, \\ &b_2(V)=\frac{c_3\phi_2(V)-2\phi_3(V)}{c_2c_3-c_2^2}, \qquad b_3(V)=\frac{c_2\phi_2(V)-2\phi_3(V)}{c_2c_3-c_3^2}, \\ &\bar{b}_1(V)=\frac{c_2c_3\phi_2(V)-(c_2+c_3)\phi_3(V)+2\phi_4(V)}{c_2c_3}, \\ &\bar{b}_2(V)=\frac{c_3\phi_3(V)-2\phi_4(V)}{c_2c_3-c_2^2}, \qquad \bar{b}_3(V)=\frac{c_2\phi_3(V)-2\phi_4(V)}{c_2c_3-c_3^2}, \\ &\bar{a}_{21}(V)=c_2^2\phi_2\big(c_2^2V\big), \qquad \bar{a}_{31}(V)=c_3^2\phi_2\big(c_3^2V\big)-\bar{a}_{32}(V), \\ &\bar{a}_{32}(V)=(c_2-c_3)c_3\phi_4(V)\big[c_2\big(c_2\phi_2(V)-2\phi_3(V)\big)\big]^{-1}. \end{aligned} \tag{30}$$

In what follows we select the free parameters c_2 and c_3. Consider (see Definition 2.7)

$$\phi=H-\arccos\left(\frac{\operatorname{tr}(S(V,z))}{2\sqrt{\det(S(V,z))}}\right), \qquad d=1-\sqrt{\det\big(S(V,z)\big)}, \tag{31}$$

where $z=\frac{\epsilon}{\omega^2+\epsilon}H^2$, $V=\frac{\omega^2}{\omega^2+\epsilon}H^2$. Since ω represents an estimation of the dominant frequency λ and $\epsilon=\lambda^2-\omega^2$ is the error of the estimation, we assume that $\epsilon=0$. Then (31) only depends on H. The parameters c_2 and c_3 are chosen such that the coefficients of the first terms in the Taylor expansions of $\phi(H)$ and $d(H)$ of the explicit ERKN integrator are minimal simultaneously. This yields

$$c_2=\frac{6-\sqrt{6}}{10}, \qquad c_3=\frac{6+\sqrt{6}}{10}. \tag{32}$$

In this case, the formulas (30) and (32) determine a three-stage explicit multi-frequency and multidimensional ERKN integrator of order three with minimal dispersion error and dissipation error. We denote the above method as MERKN3s3. The Taylor series expansions of these coefficients are

$$\begin{aligned} &b_1(V)=\frac{1}{9}I-\frac{1}{18}V+\frac{31}{7560}V^2-\frac{1}{8505}V^3+\cdots, \\ &b_2(V)=\frac{16+\sqrt{6}}{36}I+\frac{-8-3\sqrt{6}}{144}V+\frac{64+29\sqrt{6}}{30\,240}V^2+\frac{-88-43\sqrt{6}}{2\,177\,280}V^3+\cdots, \end{aligned}$$

$$b_3(V)=\left(\frac{4}{9}-\frac{1}{6\sqrt{6}}\right)I+\frac{-8+3\sqrt{6}}{144}V+\frac{64-29\sqrt{6}}{30\,240}V^2+\frac{-88+43\sqrt{6}}{2\,177\,280}V^3+\cdots,$$
$$\bar{b}_1(V)=\frac{1}{9}I-\frac{19}{1080}V+\frac{23}{30\,240}V^2-\frac{17}{1\,088\,640}V^3+\cdots,$$
$$\bar{b}_2(V)=\frac{7+2\sqrt{6}}{36}I+\frac{26-11\sqrt{6}}{2160}V+\frac{19+9\sqrt{6}}{60\,480}V^2+\frac{-2-\sqrt{6}}{435\,456}V^3+\cdots,$$
$$\bar{b}_3(V)=\frac{7-2\sqrt{6}}{36}I+\frac{26+11\sqrt{6}}{2160}V+\frac{19-9\sqrt{6}}{60\,480}V^2+\frac{-2+\sqrt{6}}{435\,456}V^3+\cdots,$$
$$\bar{a}_{21}(V)=-\frac{3(-7+2\sqrt{6})}{100}I+\frac{3(-73+28\sqrt{6})}{20\,000}V-\frac{3(-847+342\sqrt{6})}{10\,000\,000}V^2+\frac{9(-10\,033+4088\sqrt{6})}{28\,000\,000\,000}V^3+\cdots,$$
$$\bar{a}_{31}(V)=\frac{3+8\sqrt{6}}{500}I+\frac{-4809+176\sqrt{6}}{300\,000}V+\frac{-52\,587+25\,018\sqrt{6}}{42\,000\,000}V^2+\frac{-54\,347\,217+22\,468\,088\sqrt{6}}{252\,000\,000\,000}V^3+\cdots,$$
$$\bar{a}_{32}(V)=\frac{51+11\sqrt{6}}{250}I+\frac{381-359\sqrt{6}}{75\,000}V+\frac{39\,537-12\,943\sqrt{6}}{26\,250\,000}V^2+\frac{3\,345\,909-1\,424\,951\sqrt{6}}{15\,750\,000\,000}V^3+\cdots.$$

Remark 5.1. In the numerical experiments in Section 6, we use these Taylor expansions (the first four terms) to evaluate the coefficients of the method MERKN3s3.

With regard to the coefficients in the method MERKN3s3, we have the following result.

Proposition 5.2. *The coefficients of the method MERKN3s3 satisfy Assumption 3.3.*

Proof. It is trivial to show that these coefficients are bounded for a given matrix M. In the follows we prove that these coefficients are uniformly bounded for any symmetric and positive semi-definite matrix M. By Proposition 2.1(ii), it is true that $\|\phi_l(V)\|$ $(l=0,1,\dots,$ and $V=h^2M)$ are uniformly bounded with respect to a symmetric and positive semi-definite matrix M, and so are the coefficients given in (30) except $\bar{a}_{31}(V)$ and $\bar{a}_{32}(V)$.

With regard to the coefficient $\bar{a}_{32}(V)$, following the analysis in the proof of Proposition 2.1, we obtain

$$\bar{a}_{32}(V)=P^T\big(\tilde{f}(hW)\big)P,$$

where

$$\tilde{f}(x)=-\big((-39+4\sqrt{6})x^2+3(-7+2\sqrt{6})x^2\cos(x)-10(-6+\sqrt{6})x\sin(x)\big)^{-1}$$
$$\big(3(1+\sqrt{6})\big(-2+x^2+2\cos(x)\big)\big),\quad x\geqslant 0.$$

From the fact that

$$\max_{x\geqslant 0}\big(\tilde{f}(x)\big)=0.453963483788869,\qquad \min_{x\geqslant 0}\big(\tilde{f}(x)\big)=0.256019841470057,$$
$$\tilde{f}(0)=3(1+\sqrt{6})(-6+16\sqrt{6})^{-1},$$
$$3(1+\sqrt{6})\big(10(6-\sqrt{6})\big)^{-1}\leqslant\lim_{x\to\infty}\tilde{f}(x)\leqslant 3(1+\sqrt{6})\big(2(9+\sqrt{6})\big)^{-1},$$
$$(-39+4\sqrt{6})x^2+3(-7+2\sqrt{6})x^2\cos(x)-10(-6+\sqrt{6})x\sin(x)<0\quad\text{for any } x>0,$$

it follows that $\tilde{f}(hW)$ is uniformly bounded with respect to W. Thus $\bar{a}_{32}(V)$ is uniformly bounded with respect to a symmetric and positive semi-definite matrix M, and so is $\bar{a}_{31}(V)$. □

The dispersion error and dissipation error of the method MERKN3s3 are

$$\phi(H)=-\frac{(-7+2\sqrt{6})\epsilon^2}{160(2+3\sqrt{6})(\epsilon+\omega^2)^2}H^5+O\big(H^6\big);$$
$$d(H)=-\frac{\epsilon(50(-82+27\sqrt{6})\epsilon^2+125(-26+9\sqrt{6})\epsilon\omega^2+6(2+3\sqrt{6})\omega^4)}{144\,000(2+3\sqrt{6})(\epsilon+\omega^2)^3}H^6+O\big(H^7\big),$$

respectively.

Hence, the method is dispersive of order 4 and dissipative of order 5. The stability region of the method MERKN3s3 is plotted in Fig. 1 (we show only the region within $|z|\leqslant 1$ and $0\leqslant V\leqslant 10\,000$).

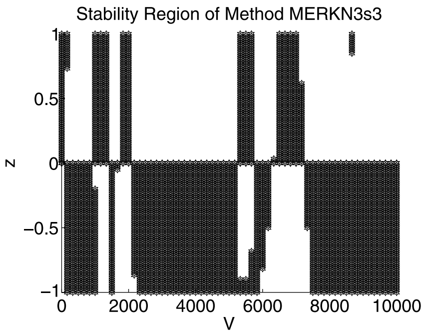

Fig. 1. Stability region (shaded region) for the method MERKN3s3.

6. Numerical experiments

Our aim in this section is to demonstrate the efficiency of the new method MERKN3s3 based on the error analysis. The methods chosen for comparison are:

- A: the symmetric Gautschi's method of order two given in [6];
- B: the symmetric Gautschi's method of order two given in [17];
- C: the symmetric Gautschi's method of order two given in [12];
- ARKN3s4: the three-stage explicit ARKN method of order four given in [28];
- RKN3s4: the three-stage explicit RKN method of order four given in [14];
- W1ERKN3s3: the three-stage explicit ERKN integrator of order three given in [30];
- W2ERKN3s3: the three-stage explicit ERKN integrator of order three given in [30];
- MERKN3s3: the three-stage explicit ERKN integrator of order three derived in this paper.

Problem 1. Consider the nonlinear wave equation (see [23])

$$\begin{cases} \dfrac{\partial^2 u}{\partial t^2} - gd(x)\dfrac{\partial^2 u}{\partial x^2} = \dfrac{1}{4}\lambda^2(x,u)u, \quad 0 < x \leqslant b,\ t > 0, \\ \dfrac{\partial u}{\partial x}(t,0) = \dfrac{\partial u}{\partial x}(t,b) = 0, \qquad u(0,x) = \sin\left(\dfrac{\pi x}{b}\right), \qquad u_t(0,x) = -\dfrac{\pi}{b}\sqrt{gd(x)}\cos\left(\dfrac{\pi x}{b}\right), \end{cases}$$

where $d(x)$ represents the depth function given by $d(x) = d_0[2 + \cos(\frac{2\pi x}{b})]$, g denotes the acceleration of gravity, and $\lambda(x,u)$ is the coefficient of bottom friction defined by $\lambda(x,u) = \frac{g|u|}{C^2 d(x)}$ with Chezy coefficient C.

By using second-order symmetric differences, this problem is converted into a system of ODEs in time

$$\begin{cases} \dfrac{d^2 U}{dt^2} + MU = F(t,U), \quad 0 < t \leqslant t_{end}, \\ U(0) = \left(\sin\left(\dfrac{\pi x_1}{b}\right), \dots, \sin\left(\dfrac{\pi x_N}{b}\right)\right)^T, \\ U'(0) = \left(-\dfrac{\pi}{b}\sqrt{gd(x_1)}\cos\left(\dfrac{\pi x_1}{b}\right), \dots, -\dfrac{\pi}{b}\sqrt{gd(x_N)}\cos\left(\dfrac{\pi x_N}{b}\right)\right)^T, \end{cases} \tag{33}$$

where $U(t)$ denotes the N-dimensional vector with entries $u_i(t) \approx u(x_i,t)$, $x_i = i\Delta x$, $\Delta x = \frac{1}{N}$,

$$M = \frac{-g}{\Delta x^2}\begin{pmatrix} -2d(x_1) & d(x_1) & & & \\ d(x_2) & -2d(x_2) & d(x_2) & & \\ & \ddots & \ddots & \ddots & \\ & & d(x_{N-1}) & -2d(x_{N-1}) & d(x_{N-1}) \\ & & & d(x_N) & -2d(x_N) \end{pmatrix},$$

and

$$F(t,U) = \left(\frac{1}{4}\lambda^2(x_1,u_1)u_1, \dots, \frac{1}{4}\lambda^2(x_N,u_N)u_N\right)^T.$$

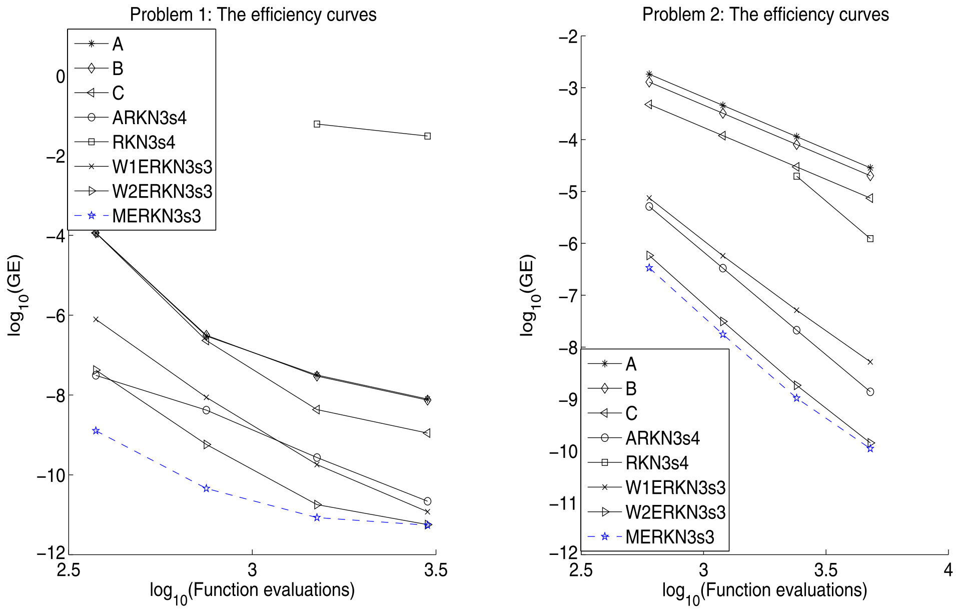

Fig. 2. Results for Problem 1 (left figure) and Problem 2 (right figure): The number of function evaluations (in logarithmic scale) against $\log_{10}(\mathrm{GE})$, the logarithm of the global error over the integration interval.

Remark 6.1. The key point should be noted here is that the matrix M in this problem is nonsymmetric. This matrix M is diagonalizable and the largest eigenvalue is about 40.093716959522474. We use this problem to show that the error analysis presented in this paper and the method MERKN3s3 are applicable for (1) with nonsymmetric M.

For the parameters in this problem we choose $b = 100$, $g = 9.81$, $d_0 = 10$, $C = 50$. The system is integrated in the interval $t \in [0, 100]$ with $N = 20$ and the stepsizes $h = 0.8/2^j$, $j = 0, 1, 2, 3$ for the three-stage methods and stepsizes $h = 0.8/(3 \times 2^j)$, $j = 0, 1, 2, 3$ for the two-stage methods. The efficiency curves (accuracy versus the computational cost measured by the number of function evaluations required by each method) are shown in Fig. 2 (left). It is noted that in these three experiments, we apply the method W1ERKN3s3 to the considered system with a smaller stepsize and consider the result as the exact solution of the system. For the RKN3s4 method, the errors are very large when $h = 0.8, 0.4$, hence we do not plot the points in Fig. 2 (right). Similar situations are encountered in the next two problems and we deal with them in a similar way. In other words, the RKN3s4 method requires smaller stepsize. Therefore, other methods chosen for such kind of problems are more practical than RKN3s4.

Problem 2. Consider the sine-Gordon equation with periodic boundary conditions (see [5])

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

We carry out a semi-discretization on the spatial variable by using second-order symmetric differences and obtain the following system of second-order ODEs in time:

$$\frac{d^2 U}{dt^2} + MU = F(t, U), \quad 0 < t \leqslant t_{end},$$

where

$$U(t) = \big(u_1(t), \ldots, u_N(t)\big)^T \quad \text{with } u_i(t) \approx u(x_i, t), \ i = 1, 2, \ldots, N,$$

$$\Delta x = 2/N, \quad x_i = -1 + i\Delta x,$$

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

$$F(t, U) = -\sin(U) = -(\sin u_1, \ldots, \sin u_N)^T.$$

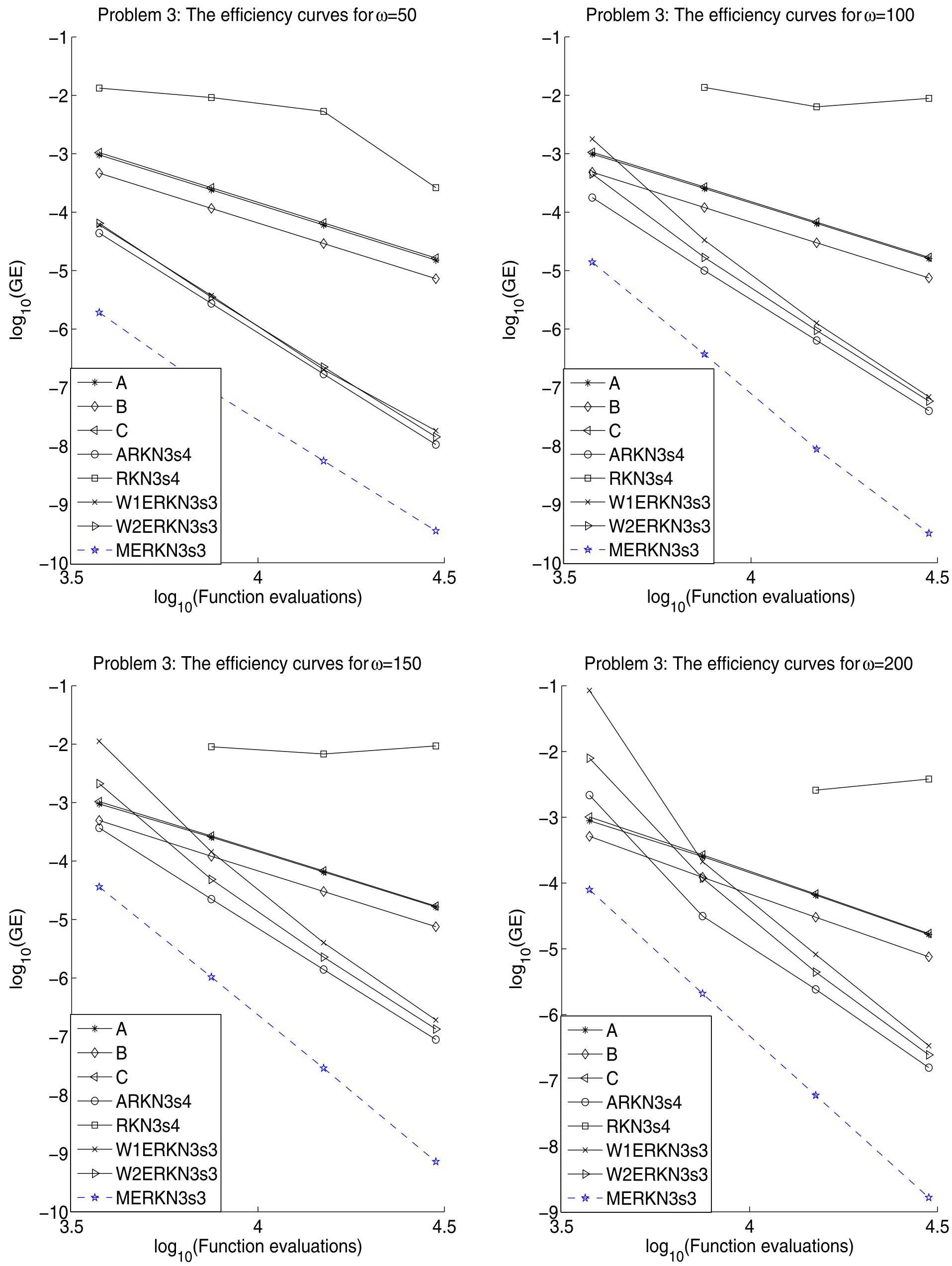

Fig. 3. Results for Problem 3 with different ω: The number of function evaluations (in logarithmic scale) against $\log_{10}(\mathrm{GE})$, the logarithm of the global error over the integration interval.

Following the paper [5], we take the initial conditions as

$$U(0) = (\pi)_{i=1}^{N}, \qquad U_t(0) = \sqrt{N}\left(0.01 + \sin\left(\frac{2\pi i}{N}\right)\right)_{i=1}^{N}.$$

Choose $N = 64$, and the problem is integrated in the interval $[0, 10]$ with stepsizes $h = 0.1/2^j$, $j = 1, 2, 3, 4$, for the three-stage methods and stepsizes $h = 0.1/(3 \times 2^j)$, $j = 1, 2, 3, 4$, for the two-stage methods. Fig. 2(right) shows the error in the positions at $t_{end} = 10$ versus the computational effort.

Problem 3. Consider a Fermi–Pasta–Ulam Problem (this problem is considered in [15,12]).

Fermi–Pasta–Ulam Problem is a Hamiltonian system with the Hamiltonian

$$H(y,x) = \frac{1}{2}\sum_{i=1}^{2m} y_i^2 + \frac{\omega^2}{2}\sum_{i=1}^{m} x_{m+i}^2 + \frac{1}{4}\left[(x_1 - x_{m+1})^4 + \sum_{i=1}^{m-1}(x_{i+1} - x_{m+i-1} - x_i - x_{m+i})^4 + (x_m + x_{2m})^4\right],$$

where x_i is a scaled displacement of the ith stiff spring, x_{m+i} represents a scaled expansion (or compression) of the ith stiff spring, and y_i, y_{m+i} are their velocities (or momenta).

Therefore, we have

$$x''(t) + Mx(t) = -\nabla U(x), \quad t \in [t_0, t_{end}],$$

where

$$M = \begin{pmatrix} \mathbf{0}_{m\times m} & \mathbf{0}_{m\times m} \\ \mathbf{0}_{m\times m} & \omega^2 I_{m\times m} \end{pmatrix},$$

$$U(x) = \frac{1}{4}\left[(x_1 - x_{m+1})^4 + \sum_{i=1}^{m-1}(x_{i+1} - x_{m+i-1} - x_i - x_{m+i})^4 + (x_m + x_{2m})^4\right].$$

Following [15], we choose

$$m = 3, \qquad x_1(0) = 1, \qquad y_1(0) = 1, \qquad x_4(0) = \frac{1}{\omega}, \qquad y_4(0) = 1,$$

with zero for the remaining initial values. The system is integrated in the interval $[0, 25]$ with stepsizes $h = 0.02/2^j$, $j = 0, 1, 2, 3$, for the three-stage methods and stepsizes $h = 0.02/(3 \times 2^j)$, $j = 0, 1, 2, 3$ for the two-stage methods. The efficiency curves for different $\omega = 50, 100, 150, 200$ are shown in Fig. 3. It can be observed from Fig. 3 that although the global errors for the methods A, B and C are independent of ω, the new method MERKN3s3 is much more accurate than these three methods.

From the numerical results of the three problems, we can conclude that the logarithm of the maximum global error of MERKN3s3 method is smaller than those of the other methods with the same numbers of the function evaluations. This indicates that MERKN3s3 is efficient and highly competitive for multi-frequency oscillatory second-order differential equations of the form (1).

7. Conclusions

In this paper, we pay attention to the error analysis for explicit multi-frequency and multidimensional ERKN integrators up to stiff order three for systems of multi-frequency oscillatory second-order differential equations (1). We analyze and present the error bounds based on a series of lemmas. *It is important to note that the theoretical analysis in this paper does not depend on the matrix decomposition of* M. That is to say, the error analysis has now been generalized from the work depending on matrix decompositions to the case where the analysis does not depend on matrix decompositions. We show that the explicit multi-frequency and multidimensional ERKN integrator fulfilling stiff order p converges with order p, and *for the important particular case where* M *is a symmetric and positive semi-definite matrix, the error bound of* $\|q_n - q(t_n)\|$ *is independent of* $\|M\|$. From the main result of error analysis, we also propose a novel explicit third order multi-frequency and multidimensional ERKN integrator with minimal dispersion error and dissipation error. The numerical experiments are performed in comparison with some well-known numerical methods in the scientific literature. It follows from the results of the numerical experiments that our new explicit third order multi-frequency and multidimensional ERKN integrator is much more efficient than various other effective methods available in the scientific literature. The error analysis in this paper clarifies the structure of the error bounds of explicit multi-frequency and multidimensional ERKN integrators. It also provides powerful means of constructing efficient ERKN integrators for the multi-frequency oscillatory system (1).

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