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Trigonometrically fitted multi-step Runge-Kutta methods for solving oscillatory initial value problems

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Abstract In this paper, trigonometrically fitted multi-step Runge-Kutta (TFMSRK) methods for the numerical integration of oscillatory initial value problems are proposed and studied. TFMSRK methods inherit the frame of multi-step Runge-Kutta (MSRK) methods and integrate exactly the problem whose solutions can be expressed as the linear combinations of functions from the set of $\{\exp(\mathrm{i}wt), \exp(-\mathrm{i}wt)\}$, or equivalently the set $\{\cos(wt), \sin(wt)\}$, where w represents an approximation of the main frequency of the problem. The general order conditions are given and four new explicit TFMSRK methods with order three and four, respectively, are constructed. Stability of the new methods is examined and the corresponding regions of stability are depicted. Numerical results show that our new methods are more efficient in comparison with other well-known high quality methods proposed in the scientific literature.

Keywords Trigonometrically fitted methods · Multi-step Runge-Kutta methods · Order conditions · Explicit methods · Oscillatory initial value problems

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1 Introduction

In this paper, we are concerned with the effective numerical integration of the initial value problem of first-order differential equations in the form

$$\begin{cases} y'(t) = f(t, y(t)), & t \in [t_0, T], \\ y(t_0) = y_0, \end{cases} \tag{1}$$

whose solution has a oscillatory character, where $y \in R^d$, $f : [t_0, T] \times R^d \to R^d$ is sufficiently differentiable. Such a problem often arises in different fields of applied sciences such as celestial mechanics, molecular dynamics, quantum mechanics, and electronics [1–4]. Regarding the oscillatory feature of the problem (1), researchers have proposed to develop integrators with frequency-dependent coefficients by some techniques like trigonometrical/exponential fitting (see [5–9]). Early presentations of these techniques are due to Gautschi [10] and Lyche [11]. Since then, a lot of exponentially fitted linear multi-step methods have been proposed. Recently, in the context of Runge-Kutta (RK) methods, exponentially fitted methods have been considered, for instance, in [12, 13], while their trigonometrically fitted version has been developed by Paternoster in [14]. All of these methods integrates exactly first-order system (1) whose solution can be expressed as linear combination of functions from the the set of functions $\{\exp(\mathrm{i}wt), \exp(-\mathrm{i}wt)\}$ or equivalently the set $\{\cos(wt), \sin(wt)\}$.

Multi-step Runge-Kutta (MSRK) methods have been developed by Burrage [15, 16]. In fact, multi-step Runge-Kutta methods belong to the class of general linear methods considered by Butcher [17]. Further more, a general class of two-step Runge-Kutta methods that depend on stage values at two consecutive steps was studied by Jackiewicz et al. [18, 19]. For further study of general two-step Runge-Kutta methods, we see [20–25]. An advantage of the MSRK methods over classical RK methods is that they can reach higher order with fewer function evaluations

Inspired by the previous work, in this paper, we will extend the idea of trigonometrical fitting to MSRK methods. The rest of this paper is organized as follows: In Section 2, we restate the general formulation of MSRK methods for the initial value problems (1). In Section 3, trigonometrical fitting conditions and algebraic order conditions for trigonometrically fitted MSRK (TFMSRK) methods are presented. In Section 4, the stability properties are analyzed. With the order conditions, four new explicit TFMSRK methods of order three and four, respectively, are constructed in Section 5. In Section 6, numerical experiments are carried out and the numerical results show the robustness of the new methods. Section 7 is concerned with conclusions and discussions.

2 Multi-step Runge-Kutta methods

Multi-step Runge-Kutta (MSRK) methods for the first-order differential system (1) are given in the following definition (see [15, 16]).

Definition 1 An s-stage l-step Runge-Kutta method for the numerical integration of the problem (1) is defined as

$$\begin{cases} Y_i = \sum_{k=1}^{l} u_{ik} y_{n-k+1} + h \sum_{j=1}^{s} a_{ij} f\left(t_n + c_j h, Y_j\right), \quad i = 1, \cdots, s, \\ y_{n+1} = \sum_{k=1}^{l} \eta_k y_{n-k+1} + h \sum_{i=1}^{s} b_i f\left(t_n + c_i h, Y_i\right), \end{cases} \tag{2}$$

where c_i, u_{ik}, a_{ij}, η_k, and b_i with $i, j = 1, \cdots, s$, $k = 1, \cdots, l$ are all real coefficients.

The method (2) can also be expressed briefly in the Butcher-type tableau as

$$\begin{array}{c|c|c} c & U & A \\ \hline & \eta^T & b^T \end{array} = \begin{array}{c|ccc|ccc} c_1 & u_{11} & \cdots & u_{1l} & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ c_s & u_{s1} & \cdots & u_{sl} & a_{s1} & \cdots & a_{ss} \\ \hline & \eta_1 & \cdots & \eta_l & b_1 & \cdots & b_s \end{array}$$

or equivalently by the quintuplet (c, U, A, η, b). In the rest of this paper, under the following conditions

$$\sum_{k=1}^{l} u_{ik} = 1, \quad \sum_{k=1}^{l} \eta_k = 1, \tag{3}$$

we restrict ourselves to the autonomous case of the form

$$\begin{cases} y'(t) = f(y(t)), \quad t \in [t_0, T], \\ y(t_0) = y_0. \end{cases} \tag{4}$$

The conditions for an MSRK method (2) to have algebraic order of accuracy p have been investigated in [4, 15, 16] by using the theory of B-series. Firstly, the reader is referred to those references for all the definitions and notations. As it is usual in the case of RK methods, the local truncation error can be expanded in the form

$$y(t_{n+1}) - y_{n+1} = \sum_{t \in T} \frac{h^{\rho(t)}}{\rho(t)!} \alpha(t) \left(1 - \sum_{k=1}^{l} \eta_k (1-k)^{\rho(t)} - \sum_{i=1}^{s} b_i \psi_i'(t)\right) F(t)(y(t_n)), \tag{5}$$

where the values $\psi_i'(t)$ are given recursively by

$$\psi_i(t) = \sum_{k=1}^{l} \eta_k (1-k)^{\rho(t)} + \sum_{j=1}^{s} a_{ij} \psi_j'(t),$$

and

$$\begin{array}{l} \psi_j'(\emptyset) = 0, \quad \psi_j'(\tau) = 1, \\ \psi_j'(t) = \rho(t) \prod_{i=1}^{m} \psi_j(t_i), \quad for\ t = [t_1, \cdots, t_m] \in T. \end{array} \tag{6}$$

The set T of rooted trees t, functions $\rho(t)$, $\alpha(t)$ and $F(t)(y)$ are defined in [3, 4]. Therefore, we restate the conditions for an MSRK method having order p as follows

Theorem 1 *For exact starting values (the local assumptions) $y_{n-k+1} = y(t_n+(-k+1)h)$, $k = 1, \cdots, l$, the MSRK method (2) is convergent of order p if and only if*

$$1 = \sum_{k=1}^{l} \eta_k (1-k)^{\rho(t)} + \sum_{i=1}^{s} b_i \psi_i'(t), \tag{7}$$

where $\rho(t) \leq p$ and $t \in T$.

3 Trigonometrically fitting conditions and order conditions

The idea of constructing methods which integrate exactly a set of linearly independent functions different of the polynomials has been proposed by several authors [12, 13]. This idea consists of selecting the available parameter of MSRK method (2) in order to make the method exact for a linear space of functions with basis

$$\mathcal{F} = \langle\, \varphi_1(t), \varphi_2(t), \cdots, \varphi_r(t) \,\rangle, \quad r \leq s.$$

In such case, the following conditions should be satisfied

$$\begin{aligned}
&\varphi_m(t_n + c_i h) = \sum_{k=1}^{l} u_{ik} \varphi_m(t_n + (-k+1)h) + h \sum_{j=1}^{s} a_{ij} \varphi_m'(t_n + c_j h),\\
&\qquad i = 1, \cdots, s, \quad m = 1, \cdots, r,\\
&\varphi_m(t_n + h) = \sum_{k=1}^{l} \eta_k \varphi_m(t_n + (-k+1)h) + h \sum_{i=1}^{s} b_i \varphi_m'(t_n + c_i h), \quad m = 1, \cdots, r.
\end{aligned}$$

When $\mathcal{F}$ contains only polynomial functions up to a certain degree ($u_m(t) = t^{m+1}$) the corresponding methods are the standard multi-step Runge-Kutta methods. Here, we consider the following exponential functions as reference set of functions:

$$\mathcal{F}_1 = \langle\, \exp(\mathrm{i}wt), \exp(-\mathrm{i}wt) \,\rangle, \quad \text{with} \quad \mathrm{i}^2 = -1.$$

This leads to the following equations

$$\begin{aligned}
&\exp(\pm \mathrm{i} c_i v) = \sum_{k=1}^{l} u_{ik} \exp(\pm \mathrm{i}(1-k)v) \pm \mathrm{i}v \sum_{j=1}^{s} a_{ij} \exp(\pm \mathrm{i} c_j v), \quad i = 1, \cdots, s,\\
&\exp(\pm \mathrm{i} v) = \sum_{k=1}^{l} \eta_k \exp(\pm \mathrm{i}(1-k)v) \pm \mathrm{i}v \sum_{i=1}^{s} b_i \exp(\pm \mathrm{i} c_i v), \quad v = wh.
\end{aligned} \tag{8}$$

With the Euler formula $\exp(\pm \mathrm{i}v) = \cos(v) \pm \mathrm{i}\sin(v)$, (9) are equivalent to the following trigonometrical fitting (TF) conditions:

$$\begin{aligned}
\sin(c_i v) &= \sum_{k=1}^{l} u_{ik} \sin((1-k)v) + v \sum_{j=1}^{s} a_{ij} \cos(c_j v), \\
\cos(c_i v) &= \sum_{k=1}^{l} u_{ik} \cos((1-k)v) - v \sum_{j=1}^{s} a_{ij} \sin(c_j v), \quad i = 1, \cdots, s, \\
\sin(v) &= \sum_{k=1}^{l} \eta_k \sin((1-k)v) + v \sum_{i=1}^{s} b_i \cos(c_i v), \\
\cos(v) &= \sum_{k=1}^{l} \eta_k \cos((1-k)v) - v \sum_{i=1}^{s} b_i \sin(c_i v).
\end{aligned} \tag{9}$$

An MSRK method (2) satisfying the TF conditions (9) will be called a trigonometrically fitted MSRK (TFMSRK) method.

Now we study the order of accuracy for TFMSRK methods. In order to analyze the conditions so that the local truncation error satisfies

$$y(t_n + h) - y_{n+1} = O(h^{p+1}),$$

we must have in mind that u_{ik}, a_{ij}, η_k, and b_i also vary as the functions of the stepsize (they vary as functions of $v = wh$). So we have the following theorem on the algebraic order.

Theorem 2 *For exact starting values (the local assumptions)* $y_{n-k+1} = y(t_n + (-k+1)h),\ k = 1, \cdots, l$, *the TFMSRK method* (2) *is convergent of order* p *if and only if*

$$1 = \sum_{k=1}^{l} \eta_k (1-k)^{\rho(t)} + \sum_{i=1}^{s} b_i \psi_i'(t) + O(v^{p+1-\rho(t)}), \tag{10}$$

where $\rho(t) \leq p$ *and* $t \in T$.

Proof The "if" part is an immediate consequence of (5) and (10). Next we prove the "only if" part. If a TFMSRK method is convergent of order p, the conditions (5) imply that

$$1 - \sum_{k=1}^{l} \eta_k (1-k)^{\rho(t)} - \sum_{i=1}^{s} b_i \psi_i'(t) = O(h^{p+1-\rho(t)}), \tag{11}$$

for $\rho(t) \leq p$ and $t \in T$. In the conditions (11), η_k, b_i, and ψ_i depend on $v = wh$, which means that w and h appear in the form v. So the result is achieved. □

Remark 1 As it may be observed, when the parameter $v = hw \to 0$, conditions (10) become the same as the standard conditions (7) for p-th order multi-step Runge-Kutta methods.

Remark 2 When p becomes bigger, the number of independent conditions to be satisfied for order p becomes larger. In this case, the simplifying conditions

$$\sum_{j=1}^{s} a_{ij} c_j^{\alpha} = \frac{1}{\alpha+1}\left(c_i^{\alpha+1} - \sum_{k=1}^{l} u_{ik}(1-k)^{\alpha+1}\right), \quad \alpha = 0, 1, 2, \cdots \tag{12}$$

can reduce the number of independent order conditions. The first and most important simplifying condition is

$$\sum_{j=1}^{s} a_{ij} = c_i - \sum_{k=1}^{l} u_{ik}(1-k).$$

For more simplifying conditions, we see [4, 15, 16].

Now we list the p-th order conditions (10) up to trees with $\rho(t) \leq 4$.

- For the SN-trees τ ($\rho(\tau) = 1$) and t with $\rho(t) = 2$, we have
$\sum_{i=1}^{s} b_i = 1 - \sum_{k=1}^{l} \eta_k(1-k) + O(v^p)$,
$\sum_{i=1}^{s} b_i \left(\sum_{k=1}^{l} u_{ik}(1-k) + \sum_{j=1}^{s} a_{ij}\right) = \frac{1}{2}\left(1 - \sum_{k=1}^{l} \eta_k(1-k)^2\right) + O(v^{p-1})$.
- For the SN-trees t with $\rho(t) = 3$, we have
$\sum_{i=1}^{s} b_i \left(\sum_{k=1}^{l} u_{ik}(1-k) + \sum_{j=1}^{s} a_{ij}\right)^2 = \frac{1}{3}\left(1 - \sum_{k=1}^{l} \eta_k(1-k)^3\right) + O(v^{p-2})$,
$\sum_{i=1}^{s} b_i \left(\sum_{k=1}^{l} u_{ik}(1-k)^2 + 2\sum_{j=1}^{s} a_{ij}\left(\sum_{k=1}^{l} u_{jk}(1-k) + \sum_{k=1}^{s} a_{jk}\right)\right)$
$= \frac{1}{3}\left(1 - \sum_{k=1}^{l} \eta_k(1-k)^3\right) + O(v^{p-2})$.
- For the SN-trees t with $\rho(t) = 4$, we have
$\sum_{i=1}^{s} b_i \left(\sum_{k=1}^{l} u_{ik}(1-k) + \sum_{j=1}^{s} a_{ij}\right)^3 = \frac{1}{4}\left(1 - \sum_{k=1}^{l} \eta_k(1-k)^4\right) + O(v^{p-3})$,
$\sum_{i=1}^{s} b_i \left(\sum_{k=1}^{l} u_{ik}(1-k) + \sum_{j=1}^{s} a_{ij}\right)\left(\sum_{k=1}^{l} u_{ik}(1-k)^2 + 2\sum_{j=1}^{s} a_{ij}\left(\sum_{k=1}^{l} u_{jk}(1-k) + \sum_{k=1}^{s} a_{jk}\right)\right)$
$= \frac{1}{4}\left(1 - \sum_{k=1}^{l} \eta_k(1-k)^4\right) + O(v^{p-3})$,
$\sum_{i=1}^{s} b_i \left(\sum_{k=1}^{l} u_{ik}(1-k)^3 + 3\sum_{j=1}^{s} a_{ij}\left(\sum_{k=1}^{l} u_{jk}(1-k) + \sum_{k=1}^{s} a_{jk}\right)^2\right)$
$= \frac{1}{4}\left(1 - \sum_{k=1}^{l} \eta_k(1-k)^4\right) + O(v^{p-3})$,
$\sum_{i=1}^{s} b_i \left(\sum_{k=1}^{l} u_{ik}(1-k)^3 + 3\sum_{j=1}^{s} a_{ij}\left(\sum_{k=1}^{l} u_{jk}(1-k)^2 + 2\sum_{k=1}^{s} a_{jk}\left(\sum_{q=1}^{l} u_{kq}(1-q) + \sum_{q=1}^{s} a_{kq}\right)\right)\right)$
$= \frac{1}{4}\left(1 - \sum_{k=1}^{l} \eta_k(1-k)^4\right) + O(v^{p-3})$.

To end this section, we present some properties related with the algebraic order reached by the TFMSRK methods.

Proposition 1 *An TFMSRK method satisfies the following relations*

$$\begin{aligned}
\sum_{i=1}^{s} b_i &= 1 - \sum_{k=1}^{l} \eta_k (1-k) + O(v^2),\\
\sum_{i=1}^{s} b_i c_i &= \tfrac{1}{2}\left(1 - \sum_{k=1}^{l} \eta_k (1-k)^2\right) + O(v^2),\\
\sum_{j=1}^{s} a_{ij} &= c_i - \sum_{k=1}^{l} u_{ik} (1-k) + O(v^2),\\
\sum_{j=1}^{s} a_{ij} c_j &= \tfrac{1}{2}\left(c_i^2 - \sum_{k=1}^{l} u_{ik} (1-k)^2\right) + O(v^2).
\end{aligned} \tag{13}$$

Proof First of all, we prove the second expression. Using the final condition given in (9) and express the trigonometric function, we have

$$\sum_{m=0}^{\infty} \frac{(-1)^m v^{2m}}{(2m)!}\left(1 - \sum_{k=1}^{l} \eta_k (1-k)^{2m}\right) = \sum_{m=0}^{\infty} \frac{(-1)^m v^{2m}}{(2m+1)!}\left(-v^2 \sum_{i=1}^{s} b_i c_i^{2m+1}\right).$$

With (3) in mind, the above formula can be expressed as

$$\begin{aligned}
&-\tfrac{v^2}{2}\left(1 - \sum_{k=1}^{l} \eta_k (1-k)^2\right) + \sum_{m=2}^{\infty} \tfrac{(-1)^m v^{2m}}{(2m)!}\left(1 - \sum_{k=1}^{l} \eta_k (1-k)^{2m}\right)\\
&= -v^2 \sum_{i=1}^{s} b_i c_i + \sum_{m=1}^{\infty} \tfrac{(-1)^m v^{2m}}{(2m)!}\left(-v^2 \sum_{i=1}^{s} b_i c_i^{2m}\right),
\end{aligned}$$

and therefore,

$$\sum_{i=1}^{s} b_i c_i = \frac{1}{2}\left(1 - \sum_{k=1}^{l} \eta_k (1-k)^2\right) + O(v^2).$$

The other expressions can be proved in a similar way. □

Proposition 2 *An TFMSRK method satisfies the following relations*

$$\sum_{i=1}^{s} b_i \left(\sum_{k=1}^{l} u_{ik}(1-k) + \sum_{j=1}^{s} a_{ij}\right) = \frac{1}{2}\left(1 - \sum_{k=1}^{l} \eta_k (1-k)^2\right) + O(v^2).$$

and therefore it has algebraic order at least two.

Proof Combining the second and third conditions of (13) yields

$$\begin{aligned}
&\sum_{i=1}^{s} b_i \left(\sum_{k=1}^{l} u_{ik}(1-k) + \sum_{j=1}^{s} a_{ij}\right) = \sum_{i=1}^{s} b_i \left(c_i + O(v^2)\right)\\
&= \sum_{i=1}^{s} b_i c_i + O(v^2) = \frac{1}{2}\left(1 - \sum_{k=1}^{l} \eta_k (1-k)^2\right) + O(v^2).
\end{aligned}$$

From the above result and the first condition of (13), the order conditions (10) are satisfied for $p = 2$ and the TFMSRK method has algebraic order at least 2. □

4 Stability

In order to analyze the stability of TFMSRK methods in this paper, following [26], we choose to consider the following linear scalar problem

$$y'(t) = \lambda y(t), \tag{14}$$

where λ is a complex parameter such that $\mathrm{Re}(\lambda) < 0$. Applying a TFMSRK method (2) to the problem (14) yields

$$Y = \sum_{k=1}^{l} U_k y_{n-k+1} + HAY,$$
$$y_{n+1} = \sum_{k=1}^{l} \eta_k y_{n-k+1} + Hb^T Y,$$

where $H = \lambda h$ and U_k is the k-th column of the coefficient matrix U. Elimination of the vector Y delivers the recursion

$$y_{n+1} - \sum_{k=1}^{l} m_k(H, v) y_{n-k+1} = 0, \tag{15}$$

where

$$m_k(H, v) = \eta_k + Hb^T (I - HA)^{-1} U_k, \quad k = 1, \cdots, l.$$

The stability properties of TFMSRK methods (2) are determined by the characteristic equation

$$\xi^l - \sum_{k=1}^{l} m_k(H, v) \xi^{l-k} = 0. \tag{16}$$

The behavior of the numerical solution will depend on the eigenvalues $r_i(H, v)$, $i = 1, \cdots, l$ of the characteristic (16). Geometrically, the characterization of stability becomes a three-dimensional region in $(\mathrm{Re}(H), \mathrm{Im}(H), v)$ space for a TFMSRK method.

Definition 2 For the TFMSRK method (2) with the characteristic (16), the region of the three-dimensional space

$$\Omega := \{(\mathrm{Re}(H), \mathrm{Im}(H), v) : |r_k(H, v)| < 1, \quad k = 1, \cdots, l\}$$

is called the region of stability. And any closed surface defined by $\max_{1 \le k \le l} |r_k(H, v)| = 1$ is a stability boundary of the method.

Remark 3 For a TFMSRK method, the three-dimensional stability region in the$(\mathrm{Re}(H), \mathrm{Im}(H), v)$ space is not very intuitive. In this paper, we will present a selection of sections through the three-dimensional stability region by planes where v is constant.

5 Construction of explicit TFMSRK methods

In this section, we focus our attentions on the construction of the explicit TFMSRK methods. We will consider explicit TFMSRK method of the form

$$\begin{cases} Y_k = y_{n-k+l}, \quad k = 1, \cdots, l, \\ Y_i = \sum\limits_{k=1}^{l} u_{ik} y_{n-k+1} + h \sum\limits_{j=1}^{i-1} a_{ij} f\left(Y_j\right), \quad i = l+1, \cdots, s, \\ y_{n+1} = \sum\limits_{k=1}^{l} \eta_k y_{n-k+1} + h \sum\limits_{i=1}^{s} b_i f(Y_i). \end{cases} \tag{17}$$

Remark 4 We note that after the starting procedure, the methods only require the evaluation of $f(y_n)$, $f(Y_{l+1}), \cdots, f(Y_s)$ in each step ($s-l+1$ function evaluations).

As an example to demonstrate the process of constructing the algorithm, we only consider two-step Runge-Kutta (TSRK) method which under the conditions (3) can be equivalently expressed as follows:

$$\begin{cases} Y_1 = y_{n-1}, \quad Y_2 = y_n, \\ Y_i = (1-u_i) y_n + u_i y_{n-1} + h \sum\limits_{j=1}^{i-1} a_{ij} f\left(Y_j\right), \quad i = 3, \cdots, s, \\ y_{n+1} = (1-\theta) y_n + \theta y_{n-1} + h \sum\limits_{i=1}^{s} b_i f(Y_i). \end{cases} \tag{18}$$

5.1 The case of $s = 3$

The order conditions for the explicit trigonometrically fitted TSRK (TFTSRK) methods (18) of order three are

$$\begin{aligned} &\sum_{i=1}^{3} b_i = 1 + \theta + O(v^3), \\ &\sum_{i=1}^{3} b_i \left(-u_i + \sum_{j=1}^{i-1} a_{ij}\right) = \tfrac{1}{2}(1-\theta) + O(v^2), \\ &\sum_{i=1}^{3} b_i \left(-u_i + \sum_{j=1}^{i-1} a_{ij}\right)^2 = \tfrac{1}{3}(1+\theta) + O(v), \\ &\sum_{i=1}^{3} b_i \left(u_i + 2\sum_{j=1}^{i-1} a_{ij} \left(-u_j + \sum_{k=1}^{j-1} a_{jk}\right)\right) = \tfrac{1}{3}(1+\theta) + O(v). \end{aligned} \tag{19}$$

Here, we select

$$c_3 = 1, \quad u_3 = 1, \quad \theta = 1. \tag{20}$$

Using the TF conditions (9) and the following order condition

$$\sum_{i=1}^{3} b_i = 1 + \theta,$$

we obtain the coefficients as follows:

$$\begin{aligned} &a_{31} = 0, \quad a_{32} = \frac{2\sin(v)}{v}, \\ &b_1 = \frac{v - \sin(v)}{v - v\cos(v)}, \quad b_2 = 2 + \csc^2\left(\frac{v}{2}\right)\left(-1 + \frac{\sin(v)}{v}\right), \quad b_3 = b_1. \end{aligned} \tag{21}$$

It is also interesting to check the algebraic third order conditions for the method

$$\begin{aligned} &\sum_{i=1}^{3} b_i = 1 + \theta + O(v^3), \quad \sum_{i=1}^{3} b_i \left(-u_i + \sum_{j=1}^{i-1} a_{ij}\right) = \frac{1}{2}(1-\theta) - \frac{v^2}{9} + \cdots, \\ &\sum_{i=1}^{3} b_i \left(-u_i + \sum_{j=1}^{i-1} a_{ij}\right)^2 = \frac{1}{3}(1+\theta) - \frac{v^2}{5} + \cdots, \\ &\sum_{i=1}^{3} b_i \left(u_i + 2\sum_{j=1}^{i-1} a_{ij}\left(-u_j + \sum_{k=1}^{j-1} a_{jk}\right)\right) = \frac{1}{3}(1+\theta) + \frac{v^2}{45} + \cdots. \end{aligned}$$

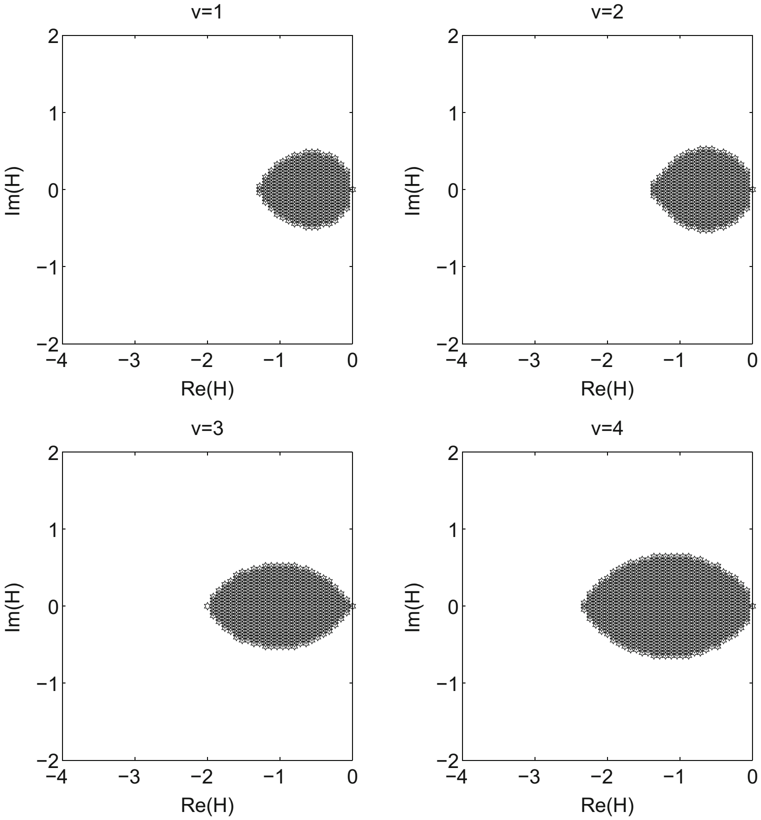

Fig. 1 Sections through the stability region for the method ETFTSRK3S by plane $v = 1, 2, 3, 4$, respectively

For small values $|v| \to 0$, the above formulae (21) are subject to heavy cancellations and in that case the following Taylor series expansions must be used:

$$\begin{aligned} &a_{31} = 0, \quad a_{32} = 2 - \tfrac{v^2}{3} + \tfrac{v^4}{60} - \tfrac{v^6}{2520} + \tfrac{v^8}{181440} + \cdots, \\ &b_1 = \tfrac{1}{3} + \tfrac{v^2}{90} + \tfrac{v^4}{2520} + \tfrac{v^6}{75600} + \tfrac{v^8}{2395008} + \cdots, \\ &b_2 = \tfrac{4}{3} - \tfrac{v^2}{45} - \tfrac{v^4}{1260} - \tfrac{v^6}{37800} - \tfrac{v^8}{1197504} + \cdots, \quad b_3 = b_1. \end{aligned} \tag{22}$$

Generally, we use the Taylor expansion (22) when $|v| < 0.01$. In the other TFMSRK methods and the other trigonometrically fitted methods in the numerical experiments of the paper, we take the same threshold about the use of the Taylor expansion.

We denote the method (18) determined by (20) and (22) as ETFTSRK3S. Sections through the stability region for the method ETFTSRK3S by plane $v = 1, 2, 3, 4$, respectively, are depicted in Fig. 1.

5.2 The case of $s = 4$

Under the first simplifying condition, the order conditions for the explicit trigonometrically fitted TSRK (TFTSRK) methods (18) of order four are reduced to

$$\begin{aligned} &\sum_{i=1}^{4} b_i = 1 + \theta + O(v^4), \quad \sum_{i=1}^{4} b_i c_i = \tfrac{1}{2}(1-\theta) + O(v^3), \\ &\sum_{i=1}^{4} b_i c_i^2 = \tfrac{1}{3}(1+\theta) + O(v^2), \quad \sum_{i=1}^{4} b_i \left(u_i + 2\sum_{j=1}^{i-1} a_{ij} c_j \right) = \tfrac{1}{3}(1+\theta) + O(v^2), \\ &\sum_{i=1}^{4} b_i c_i^3 = \tfrac{1}{4}(1-\theta) + O(v), \quad \sum_{i=1}^{4} b_i c_i \left(u_i + 2\sum_{j=1}^{i-1} a_{ij} c_j \right) = \tfrac{1}{4}(1-\theta) + O(v), \\ &\sum_{i=1}^{4} b_i \left(-u_i + 3\sum_{j=1}^{i-1} a_{ij} c_j^2 \right) = \tfrac{1}{4}(1-\theta) + O(v), \\ &\sum_{i=1}^{4} b_i \left(-u_i + 3\sum_{j=1}^{i-1} a_{ij} \left(u_j + 2\sum_{k=1}^{j-1} a_{jk} c_k \right) \right) = \tfrac{1}{4}(1-\theta) + O(v). \end{aligned} \tag{23}$$

In this subsection, we select the following parameter

$$c_4 = 1, \quad u_4 = 1, \quad \theta = 1. \tag{24}$$

Using the TF conditions (9), the first simplifying condition and the following order conditions

$$\sum_{i=1}^{4} b_i = 1 + \theta, \quad \sum_{i=1}^{4} b_i c_i = \frac{1}{2}(1-\theta),$$

we obtain the coefficients as follows

$$
\begin{aligned}
a_{31} &= \frac{-(1+c_3)v + c_3 v\cos(v) + v\cos(c_3 v) + \sin(v) + \sin(c_3 v) - \sin((1+c_3)v)}{v(-2+2\cos(v)+v\sin(v))},\\
a_{32} &= -\frac{c_3 v - (1+c_3)v\cos(v) + v\cos((1+c_3)v) + \sin(v) + \sin(c_3 v) - \sin((1+c_3)v)}{v(-2+2\cos(v)+v\sin(v))},\\
u_3 &= \frac{-1+\cos(v)+\cos(c_3 v) - \cos((1+c_3)v) - c_3 v\sin(v)}{-2+2\cos(v)+v\sin(v)},\\
a_{41} &= \cos\left(\tfrac{c_3 v}{2}\right)\csc\left(\tfrac{v}{2}\right)\csc\left(\tfrac{1}{2}(1+c_3)v\right)(v-\sin(v))\Big/ v,\\
a_{42} &= \frac{2(v\cos(v)+\sin(v)(-1+v\cot(c_3 v) - \csc(c_3 v)\sin(v)))}{v(-1+\cos(v)+\cot(c_3 v)\sin(v) - \csc(c_3 v)\sin(v))},\\
a_{43} &= \frac{2\sin(v)(-v+\sin(v))}{(v((-1+\cos(c_3 v))\sin(v) + (-1+\cos(v))\sin(c_3 v)))},
\end{aligned}
\tag{25}
$$

and

$$
b_1 = \frac{v-\sin(v)}{v - v\cos(v)},\ b_2 = 2+\csc^2\left(\frac{v}{2}\right)\left(-1+\frac{\sin(v)}{v}\right),\ b_3 = 0,\ b_4 = b_1. \tag{26}
$$

(24), (25), and (26) form a one-parameter family of explicit fourth order methods depending on c_3. It is also interesting to check the algebraic fourth order conditions for the family of methods

$$
\begin{aligned}
&\sum_{i=1}^{4} b_i = 1+\theta, \quad \sum_{i=1}^{4} b_i c_i = \tfrac{1}{2}(1-\theta), \quad \sum_{i=1}^{4} b_i c_i^2 = \tfrac{1}{3}(1+\theta) + \tfrac{v^2}{45} + \cdots,\\
&\sum_{i=1}^{4} b_i \left(u_i + 2\sum_{j=1}^{i-1} a_{ij} c_j\right) = \tfrac{1}{3}(1+\theta) + \tfrac{1}{135}(-7+10c_3)v^2 + \cdots,\\
&\sum_{i=1}^{4} b_i c_i^3 = \tfrac{1}{4}(1-\theta),\\
&\sum_{i=1}^{4} b_i c_i \left(u_i + 2\sum_{j=1}^{i-1} a_{ij} c_j\right) = \tfrac{1}{4}(1-\theta) + \tfrac{2}{27}(-1+c_3)v^2 + \cdots,\\
&\sum_{i=1}^{4} b_i \left(-u_i + 3\sum_{j=1}^{i-1} a_{ij} c_j^2\right) = \tfrac{1}{4}(1-\theta) + \tfrac{1}{90}(2-5c_3+5c_3^2)v^2 + \cdots,\\
&\sum_{i=1}^{4} b_i \left(-u_i + 3\sum_{j=1}^{i-1} a_{ij}\left(u_j + 2\sum_{k=1}^{j-1} a_{jk} c_k\right)\right) = \tfrac{1}{4}(1-\theta) + \left(\tfrac{1}{45} - \tfrac{c_3}{9}\right)v^2 + \cdots.
\end{aligned}
$$

For small values $|v| \to 0$ the above formulae (25) and (26) are subject to heavy cancellations and in that case the Taylor series expansions must be used. The choice of

$$
c_3 = \frac{1}{2} \tag{27}
$$

gives a TFTSRK method of order four with coefficients

$$
\begin{aligned}
a_{31} &= \frac{3}{8} - \frac{3v^2}{640} + \frac{19v^4}{179200} + \frac{113v^6}{86016000} + \frac{10831v^8}{264929280000} + \cdots, \\
a_{32} &= \frac{9}{8} - \frac{33v^2}{640} + \frac{89v^4}{179200} - \frac{437v^6}{86016000} - \frac{8419v^8}{264929280000} + \cdots, \\
u_3 &= 1 - \frac{9v^2}{160} + \frac{27v^4}{44800} - \frac{27v^6}{7168000} + \frac{201v^8}{22077440000} + \cdots, \\
a_{41} &= \frac{4}{9} + \frac{13v^2}{540} + \frac{257v^4}{181440} + \frac{593v^6}{7257600} + \frac{21491v^8}{4598415360} + \cdots, \\
a_{42} &= \frac{2}{3} + \frac{7v^2}{180} - \frac{11v^4}{20160} + \frac{v^6}{345600} - \frac{19v^8}{1532805120} + \cdots, \\
a_{43} &= \frac{8}{9} - \frac{17v^2}{270} - \frac{79v^4}{90720} - \frac{307v^6}{3628800} - \frac{1531v^8}{328458240} + \cdots, \\
b_1 &= \frac{1}{3} + \frac{v^2}{90} + \frac{v^4}{2520} + \frac{v^6}{75600} + \frac{v^8}{2395008} + \cdots, \\
b_2 &= \frac{4}{3} - \frac{v^2}{45} - \frac{v^4}{1260} - \frac{v^6}{37800} - \frac{v^8}{1197504} + \cdots, \quad b_3 = 0, \quad b_4 = b_1.
\end{aligned}
\tag{28}
$$

We denote the method (18) determined by (24), (27), and (28) as ETFTSRK4SL1. Sections through the stability region for the method ETFTSRK4SL1 by plane $v = 1, 2, 3, 4$, respectively, are depicted in Fig. 2.

Selecting

$$c_3 = \frac{3}{4} \tag{29}$$

gives another method of order four with the coefficients

$$
\begin{aligned}
a_{31} &= \frac{63}{64} - \frac{147v^2}{4096} + \frac{427v^4}{655360} - \frac{6517v^6}{1258291200} + \frac{123757v^8}{2214592512000} + \cdots, \\
a_{32} &= \frac{147}{64} - \frac{735v^2}{4096} + \frac{595v^4}{131072} - \frac{75257v^6}{1258291200} + \frac{947657v^8}{2214592512000} + \cdots, \\
u_3 &= \frac{81}{32} - \frac{441v^2}{2048} + \frac{1701v^4}{327680} - \frac{13629v^6}{209715200} + \frac{178569v^8}{369098752000} + \cdots, \\
a_{41} &= \frac{8}{21} + \frac{47v^2}{2520} + \frac{1331v^4}{1128960} + \frac{44537v^6}{541900800} + \frac{238481v^8}{39239811072} + \cdots, \\
a_{42} &= \frac{10}{9} - \frac{7v^2}{1080} - \frac{521v^4}{1451520} - \frac{311v^6}{33177600} - \frac{146291v^8}{588597166080} + \cdots, \\
a_{43} &= \frac{32}{63} - \frac{23v^2}{1890} - \frac{2083v^4}{2540160} - \frac{29593v^6}{406425600} - \frac{122533v^8}{21021327360} + \cdots, \\
b_1 &= \frac{1}{3} + \frac{v^2}{90} + \frac{v^4}{2520} + \frac{v^6}{75600} + \frac{v^8}{2395008} + \cdots, \\
b_2 &= \frac{4}{3} - \frac{v^2}{45} - \frac{v^4}{1260} - \frac{v^6}{37800} - \frac{v^8}{1197504} + \cdots, \quad b_3 = 0, \quad b_4 = b_1.
\end{aligned}
\tag{30}
$$

We denote the method (18) determined by (24), (29), and (30) as ETFTSRK4SL2. Sections through the stability region for the method ETFTSRK4SL2 by plane $v = 1, 2, 3, 4$, respectively, are depicted in Fig. 3.

Similarly, we take

$$c_3 = \frac{1}{3}, \tag{31}$$

and obtain

$$\begin{aligned}
a_{31} &= \frac{4}{27} + \frac{2v^4}{45927} + \frac{103v^6}{93002175} + \frac{25603v^8}{859340097000} + \cdots, \\
a_{32} &= \frac{16}{27} - \frac{4v^2}{243} + \frac{v^4}{76545} - \frac{289v^6}{186004350} - \frac{167857v^8}{5156040582000} + \cdots, \\
u_3 &= \frac{11}{27} - \frac{4v^2}{243} + \frac{13v^4}{229635} - \frac{83v^6}{186004350} - \frac{14239v^8}{5156040582000} + \cdots, \\
a_{41} &= \frac{1}{2} + \frac{7v^2}{270} + \frac{34v^4}{25515} + \frac{127v^6}{1968300} + \frac{1649v^8}{545612760} + \cdots, \\
a_{42} &= \frac{16v^2}{135} - \frac{52v^4}{25515} + \frac{101v^6}{3444525} + \frac{v^8}{136403190} + \cdots, \\
a_{43} &= \frac{3}{2} - \frac{13v^2}{90} + \frac{2v^4}{2835} - \frac{431v^6}{4592700} - \frac{551v^8}{181870920} + \cdots, \\
b_1 &= \frac{1}{3} + \frac{v^2}{90} + \frac{v^4}{2520} + \frac{v^6}{75600} + \frac{v^8}{2395008} + \cdots, \\
b_2 &= \frac{4}{3} - \frac{v^2}{45} - \frac{v^4}{1260} - \frac{v^6}{37800} - \frac{v^8}{1197504} + \cdots, \quad b_3 = 0, \quad b_4 = b_1,
\end{aligned} \tag{32}$$

We denote the method (18) determined by (24), (31), and (32) as ETFTSRK4SL3. Sections through the stability region for the method ETFTSRK4SL3 by plane $v = 1, 2, 3, 4$, respectively, are depicted in Fig. 4.

6 Numerical experiments

In this section, in order to show the competence and superiority of the new methods compared with the well-known methods in the scientific literature, we use six model problems. The criterion used in the numerical comparisons is the decimal logarithm of the global error (GE) versus the computational effort measured in the decimal logarithm of the number of function evaluations required by each method. The integrators we select for comparison are

- ETFTSRK4SL1: The four-stage explicit TFTSRK method of order four derived in Section 5 of this paper;
- ETFTSRK4SL2: The four-stage explicit TFTSRK method of order four derived in Section 5 of this paper;
- ETFTSRK4SL3: The four-stage explicit TFTSRK method of order four derived in Section 5 of this paper;

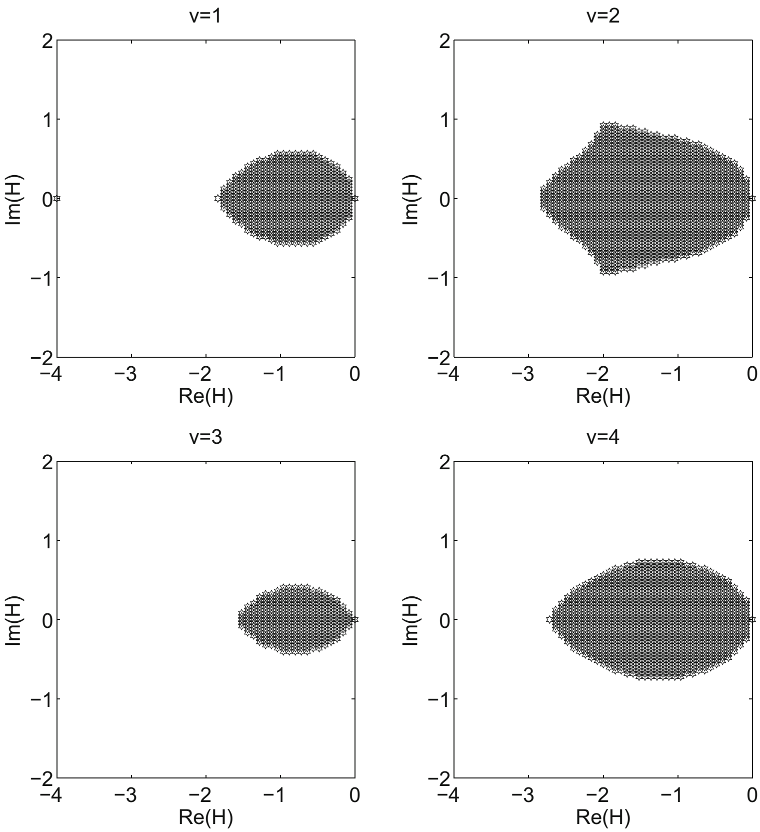

Fig. 2 Sections through the stability region for the method ETFTSRK4SL1 by plane $v = 1, 2, 3, 4$, respectively

- EFRK4B1: Exponentially fitted explicit Runge-Kutta methods of order four introduced by Vanden Berghe in [12];
- EFRK4B2: Exponentially fitted explicit Runge-Kutta methods of order four derived by Vanden Berghe in [13].
- ETSRK4SL1: The four-stage explicit two-step Runge-Kutta methods of order four underlying ETFTSRK4SL1;
- ETSRK4SL2: The four-stage explicit two-step Runge-Kutta methods of order four underlying ETFTSRK4SL2;
- ETSRK4SL3: The four-stage explicit two-step Runge-Kutta methods of order four underlying ETFTSRK4SL3;
- KUTTA4S4P1: The classical four-stage four-order explicit Runge-Kutta methods given in II.1 of [3], pp. 138;
- KUTTA4S4P2: The classical four-stage four-order explicit Runge-Kutta methods given in II.1 of [3], pp. 138.

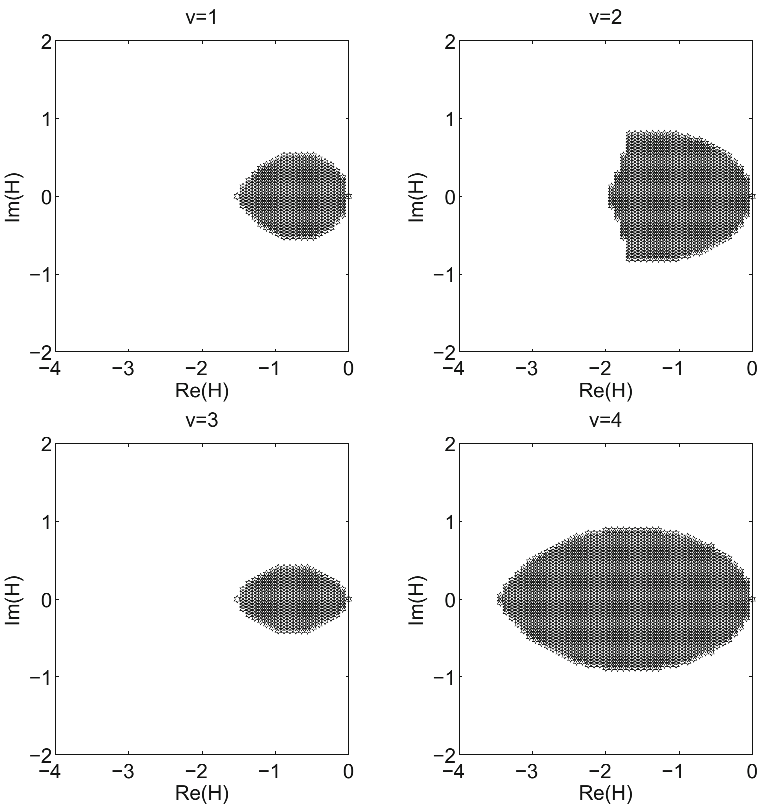

Fig. 3 Sections through the stability region for the method ETFTSRK4SL2 by plane $v = 1, 2, 3, 4$, respectively

In each step, the number of function evaluations required by ETFTSRK4SL1, ETFTSRK4SL2, ETFTSRK4SL3, ETSRK4SL1, ETSRK4SL2, and ETSRK4SL3 is three, whereas the corresponding numbers for EFRK4B1, EFRK4B2, KUTTA4S4P1, and KUTTA4S4P2 are four.

Problem 1. Consider the linear test problem used in Ref. [27]

$$y'' + w^2 y = (w^2 - 1)\sin t, \quad t \in [0, t_{end}],$$
$$y(0) = 1, \quad y'(0) = w + 1,$$

whose analytic solution is given by

$$y(t) = \cos(wt) + \sin(wt) + \sin(t).$$

In our numerical test, we choose $w = 5$ as the fitting parameter. This problem has been solved in the interval [0, 100] with the step sizes $h = 1/2^j$ for ETFTSRK4SL1, ETFTSRK4SL2, ETFTSRK4SL3, ETSRK4SL1, ETSRK4SL2, and ETSRK4SL3, $h = 1/(3 \cdot 2^{j-2})$ for EFRK4B1, EFRK4B2, KUTTA4S4P1, and KUTTA4S4P2, where $j = 3, 4, 5, 6$. The numerical results are presented in Fig. 5.

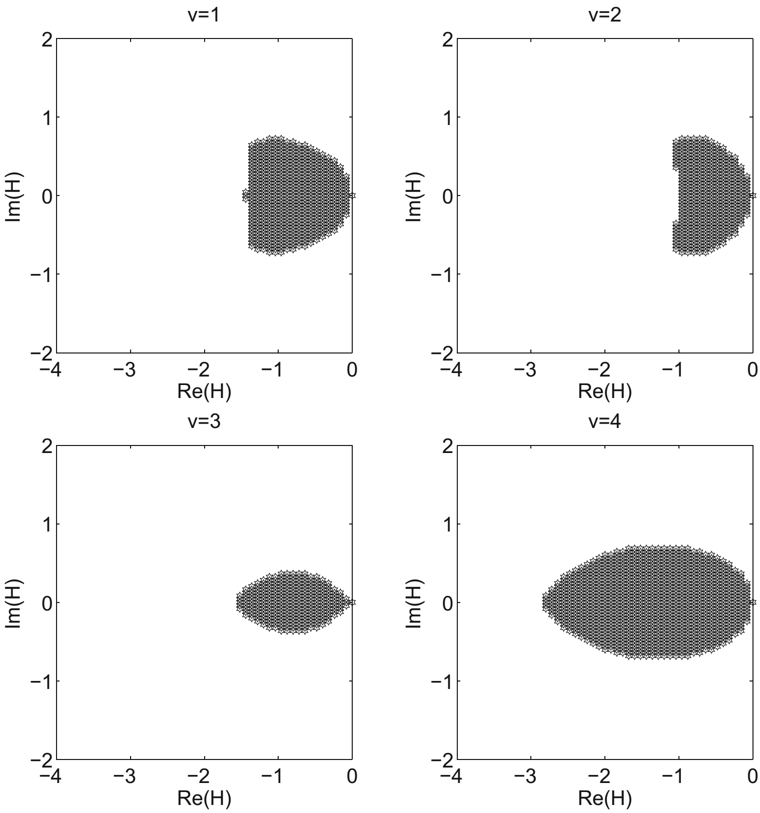

Fig. 4 Sections through the stability region for the method ETFTSRK4SL3 by plane $v = 1, 2, 3, 4$, respectively

Problem 2. Consider the linear periodic problem used in Ref. [28]

$$y'' + y = 0.001e^{\mathrm{i}t}, \quad t \in [0, t_{end}],$$
$$y(0) = 1, \quad y'(0) = 0.9995\mathrm{i},$$

with analytic solution

$$y(t) = (1 - 0.0005\mathrm{i}t)e^{\mathrm{i}t}.$$

This problem has been solved in the interval [0, 1000] with the fitting parameter $w = 1$ and the step sizes $h = 1/2^j$ for ETFTSRK4SL1, ETFTSRK4SL2, ETFTSRK4SL3, ETSRK4SL1, ETSRK4SL2, and ETSRK4SL3, $h = 1/(3 \cdot 2^{j-2})$ for EFRK4B1, EFRK4B2, KUTTA4S4P1, and KUTTA4S4P2, where $j = 0, 1, 2, 3$. The numerical results are presented in Fig. 5.

Problem 3. We consider the two-dimensional problem in [29]

$$y'' + \begin{pmatrix} 13 & -12 \\ -12 & 13 \end{pmatrix} y = \begin{pmatrix} f_1(t) \\ f_2(t) \end{pmatrix}, \quad y(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad y'(0) = \begin{pmatrix} -4 \\ 8 \end{pmatrix},$$

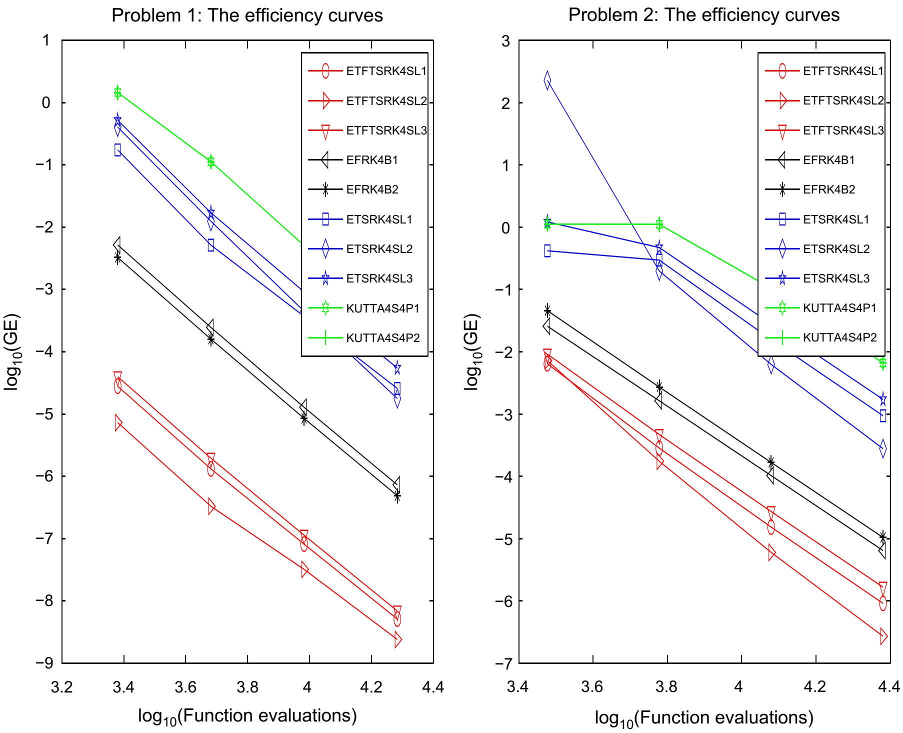

Fig. 5 Efficiency curves for Problems 1 (*left*) and 2 (*right*)

in which $f_1(t) = 9\cos(2t) - 12\sin(2t)$, $f_2(t) = 12\cos(2t) + 9\sin(2t)$, whose analytic solution is given by

$$y(t) = \begin{pmatrix} \sin(t) - \sin(5t) + \cos(2t) \\ \sin(t) - \sin(5t) + \sin(2t) \end{pmatrix}.$$

In this test, we choose $w = 5$ as the fitting parameter. This problem has been solved in the interval [0, 1000] with the step sizes $h = 1/2^j$ for ETFTSRK4SL1, ETFTSRK4SL2, ETFTSRK4SL3, ETSRK4SL1, ETSRK4SL2, and ETSRK4SL3, $h = 1/(3 \cdot 2^{j-2})$ for EFRK4B1, EFRK4B2, KUTTA4S4P1, and KUTTA4S4P2, where $j = 3, 4, 5, 6$. The numerical results are presented in Fig. 6.

Problem 4. We consider the Duffing equation

$$\begin{cases} y'' + 25y = 2k^2y^3 - k^2y, & t \in [0, t_{end}], \\ y(0) = 0, \quad y'(0) = w, \end{cases} \tag{33}$$

where $k = 0.03$. The exact solution of this initial-value problem is $y(t) = \mathrm{sn}(wt; k/w)$, the so-called Jacobian elliptic function. In this test, we choose the frequency $w = 5$ as the fitting parameter. This problem has been solved in the interval [0, 100] with the step sizes $h = 1/2^j$ for ETFTSRK4SL1, ETFTSRK4SL2, ETFTSRK4SL3, ETSRK4SL1, ETSRK4SL2, and ETSRK4SL3, $h = 1/(3 \cdot 2^{j-2})$ for

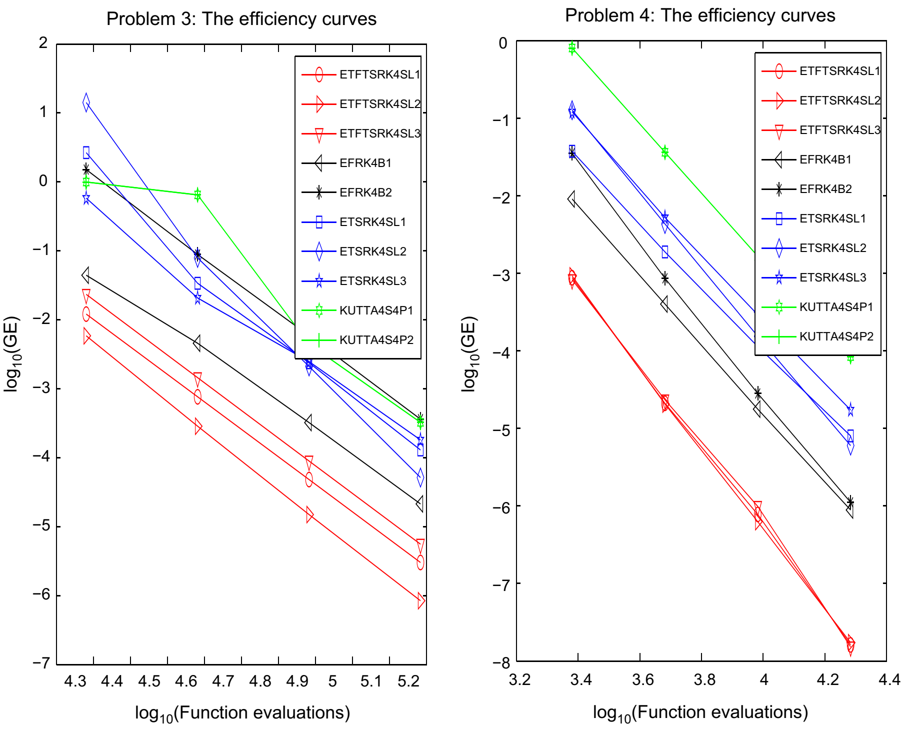

Fig. 6 Efficiency curves for Problems 3 (*left*) and 4 (*right*)

EFRK4B1, EFRK4B2, KUTTA4S4P1, and KUTTA4S4P2, where $j = 3, 4, 5, 6$. The numerical results are presented in Fig. 6.

Problem 5. A perturbed system was studied in [30]. As an example of a system we consider

$$\begin{aligned} y_1'' &= -25y_1 - \epsilon(y_1^2 + y_2^2) + \epsilon f_1(x), \quad y_1(0) = 1, \quad y_1'(0) = 0, \\ y_2'' &= -25y_2 - \epsilon(y_1^2 + y_2^2) + \epsilon f_2(x), \quad y_2(0) = \epsilon, \quad y_2'(0) = 5, \end{aligned}$$

where

$$\begin{aligned} f_1(x) &= 1 + \epsilon^2 + 2\epsilon \sin(5x + x^2) + 2\cos(x^2) + (25 - 4x^2)\sin(x^2), \\ f_2(x) &= 1 + \epsilon^2 + 2\epsilon \sin(5x + x^2) - 2\sin(x^2) + (25 - 4x^2)\cos(x^2). \end{aligned}$$

In our test, we choose $\epsilon = 10^{-3}$ and choose the frequency $w = 5$ as the fitting parameter. The analytical solution is given by:

$$y_1(x) = \cos(5x) + \epsilon \sin(x^2), \quad y_2(x) = \sin(5x) + \epsilon \cos(x^2).$$

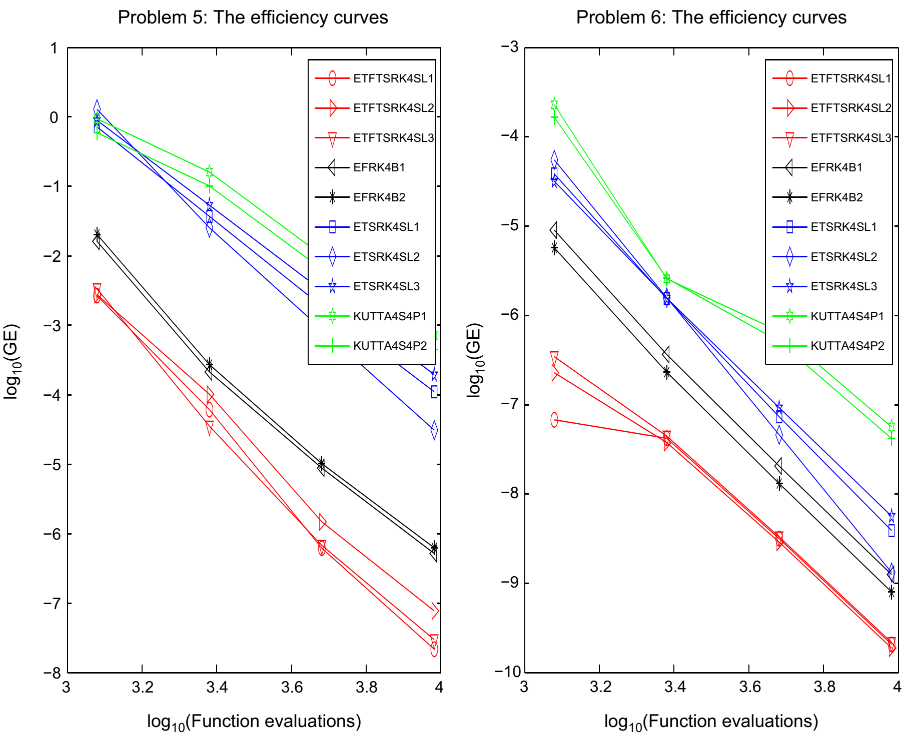

Fig. 7 Efficiency curves for Problems 5 (*left*) and 6 (*right*)

This problem has been solved in the interval [0, 100] with step sizes $h = 1/2^j$ for ETFTSRK4SL1, ETFTSRK4SL2, ETFTSRK4SL3, ETSRK4SL1, ETSRK4SL2, and ETSRK4SL3, $h = 1/(3 \cdot 2^{j-2})$ for EFRK4B1, EFRK4B2, KUTTA4S4P1, and KUTTA4S4P2, where $j = 2, 3, 4, 5$. The numerical results stated in Fig. 7.

Problem 6. Consider the periodically forced nonlinear equation governing a periodic motion of low frequency with a small perturbation of high frequency

$$\begin{cases} y'' + y = -y^3 + (\cos(x) + \sin(10x))^3 - 99\epsilon \sin(10x), \\ y(0) = 1, \quad y'(0) = 10\epsilon, \end{cases}$$

with $\epsilon = 10^{-4}$. The exact solution is

$$y(x) = \cos(x) + \epsilon \sin(10x).$$

In our test, we choose the main frequency $w = 1$ and integrate the equation in the interval [0, 100] with the step sizes $h = 1/2^j$ for ETFTSRK4SL1, ETFTSRK4SL2, ETFTSRK4SL3, ETSRK4SL1, ETSRK4SL2, and ETSRK4SL3, $h = 1/(3 \cdot 2^{j-2})$ for EFRK4B1, EFRK4B2, KUTTA4S4P1, and KUTTA4S4P2, where $j = 2, 3, 4, 5$. The numerical results are shown in Fig. 7.

7 Conclusions and discussions

We present and study trigonometrically fitted multi-step Runge-Kutta (TFMSRK) method in this paper. These methods integrates exactly first-order systems (1) whose solution can be expressed as linear combination of functions from the set of functions $\{\exp(\mathrm{i}wt), \exp(-\mathrm{i}wt)\}$, or equivalently the set $\{\cos(wt), \sin(wt)\}$. The order conditions for TFMSRK methods are derived. Based on the order conditions, four new explicit TFMSRK methods of orders three and four, respectively, are constructed. The results of the numerical experiments confirm that our new methods work more efficiently than the high quality methods we select from the scientific literature.

The determination of the frequency w for a trigonometrically fitted method is a critical issue, because the coefficients of the method depend on w. The knowledge of an estimation to the unknown frequency is needed in order to apply the numerical method efficiently. For the technique of frequency choice in trigonometrically fitted methods, the reader is referred to [31, 32].

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