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Analysis of trigonometric implicit Runge–Kutta methods

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Abstract

Using generalized collocation techniques based on fitting functions that are trigonometric (rather than algebraic as in classical integrators), we develop a new class of multistage, one-step, variable stepsize, and variable coefficients implicit Runge–Kutta methods to solve oscillatory ODE problems. The coefficients of the methods are functions of the frequency and the stepsize. We refer to this class as trigonometric implicit Runge–Kutta (TIRK) methods. They integrate an equation exactly if its solution is a trigonometric polynomial with a known frequency. We characterize the order and A-stability of the methods and establish results similar to that of classical algebraic collocation RK methods.

Keywords: Oscillatory ODEs; Variable stepsize; Variable coefficients; Trigonometric collocation; Implicit RK

1. Introduction

ODE problems that are intermittently oscillatory and/or stiff represent an important class of problems that arise in practice. In biology for example, most living organisms experience circadian (i.e., daily) oscillations that can be represented by periodic kinetics ODE models of period 24 h. Another noteworthy example is the ruby laser oscillator [2] which is difficult to solve because it is initially stiff, then mildly damped before becoming highly oscillatory, and eventually approaching a constant steady state. A number of numerical methods for oscillatory problems have been developed. Many of these methods (e.g., Runge–Kutta–Nyström) are quite generic. Some of them can however take advantage of special properties of the solution that may be known in advance. What is more rare (and harder to implement) are type-insensitive integrators that can adaptively switch between different modes of the solution (stiff, non-stiff, oscillatory).

For a periodic ODE problem whose frequency, or a reasonable estimate of it, is known in advance, it can be advantageous to tune a method to take this estimate as a prior knowledge. We describe a new class of such methods. We use generalized collocation techniques based on fitting functions that are trigonometric (rather than algebraic as in classical integrators) to develop a class of multistage, one-step, variable stepsize, and variable coefficients implicit Runge–Kutta methods to solve oscillatory ODE problems. The coefficients of the methods are functions of the frequency and the stepsize. We refer to this class as trigonometric implicit Runge–Kutta (TIRK) methods. We give the general

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forms of their coefficients and their stability functions. Although there have been similar methods constructed through the usage of a trigonometric basis, these general results are new. Moreover, we show the existence of A-stable methods in the families of the two-, three- and four-stages methods with symmetric collocation points.

The organization of the paper is as follows. We start by briefly recalling Ozawa's results in Section 2. We then define and motivate TIRK methods in Section 3. We subsequently characterize their coefficients in Section 4 and reveal their stability functions in Section 5. Finally, in Section 6 we present some numerical results and then give some concluding remarks in Section 7.

2. Functionally fitted RK methods

Classical RK methods are polynomially fitted in the sense that they integrate any ODE problem exactly if its solution is a polynomial up to some degree, though the methods have an error for general ODEs. Likewise, other RK methods relying on exponentials exist [8,9,23,24]. Extending further, Ozawa [17–19] studied a more general family of *functionally fitted* RK methods that are constructed by first choosing a set of scalar *basis functions* $\{u_k(t)\}_{k=1}^s$ that are linearly independent and sufficiently smooth, and then generating an s-stage RK method that will exactly integrate any ODE problem whose solution can be expressed as a linear combination of the basis functions. Ozawa investigated the existence of these methods. We briefly summarize his main results here since our new results build on them.

Consider the problem of solving a system of first order differential equations of dimension d

$$\begin{cases} \boldsymbol{y}'(t) = \boldsymbol{f}(t, \boldsymbol{y}(t)), & \boldsymbol{y} : \mathbb{R} \to \mathbb{R}^d, \ \boldsymbol{f} : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d, \ t \in [0, T] \\ \boldsymbol{y}(0) = \boldsymbol{y}_0 & \text{initial condition.} \end{cases} \tag{1}$$

A given s-stage RK-method is defined by its Butcher-tableau

$$\begin{array}{c|c} \boldsymbol{c} & \boldsymbol{A} \\ \hline & \boldsymbol{b}^{\mathrm{T}} \end{array}, \quad \boldsymbol{A} = (a_{ij}) \in \mathbb{R}^{s \times s}, \quad \boldsymbol{b} \in \mathbb{R}^s, \ \boldsymbol{c} = \boldsymbol{A}\boldsymbol{e}, \ \boldsymbol{e} = (1, \ldots, 1)^{\mathrm{T}},$$

in which, for an explicit RK-method, $\boldsymbol{A}$ is strictly lower triangular and $c_1 = 0$. Using the current value $\boldsymbol{y}_n$ at t_n and taking an appropriate stepsize h, the next iterate of the integration scheme is computed as

$$\begin{cases} \boldsymbol{Y}_i = \boldsymbol{y}_n + h\sum_{j=1}^s a_{ij}\boldsymbol{f}(t_n + c_j h, \boldsymbol{Y}_j), & i = 1, \ldots, s, \\ \boldsymbol{y}_{n+1} = \boldsymbol{y}_n + h\sum_{j=1}^s b_j \boldsymbol{f}(t_n + c_j h, \boldsymbol{Y}_j). \end{cases}$$

These relations are often represented compactly using a Kronecker tensor product notation. In the scalar case (i.e., $d = 1$), this becomes:

$$\boldsymbol{Y} = \boldsymbol{e} y_n + h\boldsymbol{A} f(\boldsymbol{e}t_n + \boldsymbol{c}h, \boldsymbol{Y}) \in \mathbb{R}^s,$$

$$y_{n+1} = y_n + h\boldsymbol{b}^{\mathrm{T}} f(\boldsymbol{e}t_n + \boldsymbol{c}h, \boldsymbol{Y}) \in \mathbb{R},$$

where $\boldsymbol{Y} = (Y_1, \ldots, Y_s)^{\mathrm{T}}$ and $f(\boldsymbol{e}t_n + \boldsymbol{c}h, \boldsymbol{Y}) = f(t_n + c_1 h, Y_1), \ldots, f(t_n + c_s h, Y_s)^{\mathrm{T}}$. Functionally fitted RK methods are constructed by demanding that the given scalar basis functions $\{u_k(t)\}_{k=1}^s$ satisfy the integration exactly.

Definition 1 (*Functionally fitted RK*). An s-stage RK method is a functionally fitted RK (or a generalized collocation RK) method with respect to the basis functions $\{u_k(t)\}_{k=1}^s$ if each u_k satisfies the following relations:

$$u_k(\boldsymbol{e}t + \boldsymbol{c}h) = \boldsymbol{e}u_k(t) + h\boldsymbol{A}(t, h)u_k'(\boldsymbol{e}t + \boldsymbol{c}h),$$

$$u_k(t + h) = u_k(t) + h\boldsymbol{b}(t, h)^{\mathrm{T}} u_k'(\boldsymbol{e}t + \boldsymbol{c}h). \tag{2}$$

Writing these equalities in matrix form, we get a linear system that can be solved for $\boldsymbol{A}$ and $\boldsymbol{b}$, yielding a method with variable coefficients that generally depend on t and h. The parameters $(c_i)_{i=1}^s$ are usually taken in [0, 1] and we assume that they are distinct. Ozawa [18] showed that $\boldsymbol{A}$ and $\boldsymbol{b}$ are uniquely determined for small $h > 0$ and $t \in [0, T]$ if the Wronskian $W(u_1^{(1)}, \ldots, u_s^{(1)})(t) \neq 0$. Other weaker conditions were given in [16].

Often in practice, at some time $t = t_n$, the underlying linear system to solve for the coefficients $\boldsymbol{A}$ and $\boldsymbol{b}$ tends to be ill-conditioned when $h \to 0$. But it turns out that if these coefficients are expanded into their Taylor series, their leading terms are constant and conform to implicit RK schemes [18, Corollary 1]. This shows therefore that when $h \to 0$, the functionally fitted method converges to the corresponding constant coefficient collocation method defined by $\boldsymbol{c}$. We can thus directly use the constant coefficients when $h \to 0$. Also note that while functionally fitted methods are inherently implicit, semi-implicit or diagonally implicit variants can be constructed as well by imposing a lower triangular pattern to the RK matrix [20].

As with conventional Radau-type collocation methods, these generalized s-stage collocation methods have a stage order s and an overall order at least s and at most $2s$ (see e.g., [18,16]). In particular, superconvergent methods that attain the maximum order of $2s$ can be constructed by specifically choosing the collocation parameters $(c_i)_{i=1}^s$ to satisfy some orthogonality condition, as is the case with Gauss–Legendre points.

3. Separably fitted RK methods

While generalized collocation techniques allow using arbitrary fitting functions, further refinements can be achieved when using specific functions. An immediate drawback of the generalized collocation methods is that their coefficients depend on t and h in a non-trivial manner, inhibiting any in-depth analysis of the behavior of the methods. Our own contribution in this study focuses on trigonometrically fitted RK methods that integrate any ODE problem exactly if the solution is a trigonometric polynomial. They belong to a class of methods with coefficients that are *independent* of t. We refer to this class as *separably fitted* RK methods for reasons that we shall see later. Our first new result in Theorem 2 characterizes a very general way to build these methods. We will subsequently analyze trigonometric methods in detail.

Theorem 2. *Assume that* $\{u_k\}_{k=1}^s$ *are sufficiently smooth functions that satisfy* (2) *at* 0, *i.e.*,

$$\begin{aligned} u_k(\boldsymbol{c}h) &= \boldsymbol{e}u_k(0) + h\boldsymbol{A}(0,h)u_k'(\boldsymbol{c}h), \\ u_k(h) &= u_k(0) + h\boldsymbol{b}(0,h)^{\mathrm{T}}u_k'(\boldsymbol{c}h). \end{aligned} \tag{3}$$

Assume that there exist univariate functions $\{f_{k\ell}\}$ *and* $\{g_k\}$, $k, \ell = 1, \ldots, s$, *such that*

$$u_k(x+y) = \sum_{\ell=1}^{s} f_{k\ell}(y)u_\ell(x) + g_k(y) \quad \forall x, y \in \mathbb{R}. \tag{4}$$

Then, $\{u_k\}_{k=1}^s$ *generate a functionally fitted RK method with coefficients* $(\boldsymbol{c}, \boldsymbol{b}(0,h), \boldsymbol{A}(0,h))$.

Proof. From Definition 1, we need to verify that each u_k that satisfies (3)–(4) also satisfies

$$\begin{cases} u_k(t+c_ih) = u_k(t) + h\sum_{j=1}^{s} a_{ij}(0,h)u_k'(t+c_jh), \quad i = 1, \ldots, s \\ u_k(t+h) = u_k(t) + h\sum_{j=1}^{s} b_j(0,h)u_k'(t+c_jh). \end{cases}$$

First, note that if we differentiate (4) with respect to x then

$$u_k'(x+y) = \sum_{\ell=1}^{s} f_{k\ell}(y)u_\ell'(x) \quad \forall x, y \in \mathbb{R}.$$

We can write

$$
\begin{aligned}
u_k(t+c_i h) &= \sum_{\ell=1}^{s} f_{k\ell}(t) u_\ell(c_i h) + g_k(t) \\
&= \sum_{\ell=1}^{s} f_{k\ell}(t) \left(u_\ell(0) + h \sum_{j=1}^{s} a_{ij}(0,h) u'_\ell(c_j h) \right) + g_k(t) \\
&= u_k(t) + h \sum_{j=1}^{s} a_{ij}(0,h) \sum_{\ell=1}^{s} f_{k\ell}(t) u'_\ell(c_j h) \\
&= u_k(t) + h \sum_{j=1}^{s} a_{ij}(0,h) u'_k(t+c_j h).
\end{aligned}
$$

The other equality is obtained similarly. $\square$

Remark 3. The $\{g_k\}$ in (4) vanish if one of the basis functions is constant. In other words, we can always add a constant basis function so as to fold the $\{g_k\}$ into the $\{f_{k\ell}\}$. Letting for instance $\boldsymbol{u} = (1, u_1, \ldots, u_s)^{\mathrm{T}}$, we can reformulate (4) in matrix form as

$$\boldsymbol{u}(x+y) = \mathscr{F}(y)\boldsymbol{u}(x), \tag{5}$$

where $\mathscr{F}$ is a square matrix of order $s+1$ with entries that are univariate functions.

Remark 4. Theorem 2 shows that the generalized RK coefficients depend only on h for the class of fitting functions that can be *separated* in accordance with (4) or (5). Examples include:

(1) $\{u_k(x)\}_{k=1}^{2m} = \{\sin(x), \cos(x), \ldots, \sin(mx), \cos(mx)\}$.
(2) $\{u_k(x)\}_{k=1}^{2n} = \{\sin(\omega_1 x), \cos(\omega_1 x), \ldots, \sin(\omega_n x), \cos(\omega_n x)\}$.
(3) $\{u_k(x)\}_{k=1}^{s} = \{x, \ldots, x^s\}$.
(4) $\{u_k(x)\}_{k=1}^{2m+n} = \{\sin(\omega x), \cos(\omega x), \ldots, \sin(m\omega x), \cos(m\omega x)\} \cup \{x, \ldots, x^n\}$.
(5) $\{u_k(x)\}_{k=1}^{2(n+1)} = \{\sin(\omega x), \cos(\omega x), x\sin(\omega x), x\cos(\omega x), \ldots, x^n, \sin(\omega x), x^n\cos(\omega x)\}$.
(6) $\{u_k(x)\}_{k=1}^{n+2(m+1)} = \{x, \ldots, x^n, \exp(\pm wx), x\exp(\pm wx), \ldots, x^m\exp(\pm wx)\}$.

Hence polynomials, exponentials, sine-cosine and hyperbolic sine-cosine functions, and various combinations belong to this class. We note that collocation methods based on a combination of functions of different type are also called *mixed-collocation*. In [4] for example, Coleman and Duxbury use the particular set of basis functions $\{\sin(\omega x), \cos(\omega x)\} \cup \{1, x, \ldots, x^{s-1}\}$. In our study, we simply use the terminology of trigonometric collocation to emphasize that arbitrary trigonometric terms are allowed, in the ways specified below.

Definition 5 (*TIRK*). An s-stage generalized collocation RK method is called a TIRK method if its fitting functions are $\{\sin(\omega t), \cos(\omega t), \ldots, \sin(r\omega t), \cos(r\omega t)\}$, or $\{\sin(\omega t), \cos(\omega t), \ldots, \sin(r\omega t), \cos(r\omega t)\} \cup \{t\}$, corresponding respectively to $s = 2r$ or $s = 2r+1$ basis functions, with ω being a given parameter representing the fitted frequency.

Clearly, ω is taken as the frequency of the analytical solution when it is known. But if the exact frequency is unknown or in the case of multiple frequencies, ω is assumed to be an indicative frequency chosen approximatively. We consider $(\boldsymbol{c}, \boldsymbol{b}(v), \boldsymbol{A}(v))$ as a single method whose coefficients are functions of $v = \omega h$, where ω is given in advance. Other authors, e.g. [5,3], view any such parameter-dependent method as a family of methods because ω can be deliberately set to arbitrary values once the formal Butcher tableau of the method is constructed, with each choice of ω generating a particular method. We do not overly concern ourselves with these aspects here. TIRK methods satisfy properties common to functionally fitted methods. We state these known properties here for completeness.

Theorem 6 (*Order of TIRK methods*). *An s-stage TIRK method has a stage order s and a step order at least s.*

Theorem 7 (*Superconvergence of TIRK methods*). *If an s-stage TIRK method has collocation parameters $(c_i)_{i=1}^s$ that satisfy*

$$\int_0^1 \xi^j \prod_{i=1}^s (\xi - c_i)\,\mathrm{d}\xi = 0, \quad j = 0, \ldots, q-1,$$

then the method has a step order $p = s + q$.

As noted earlier, if the $(c_i)_{i=1}^s$ are chosen as Gauss–Legendre points then the method attains the maximum order $2s$. These are known results established by Ozawa in the general case. From now on, we shall study other new properties. We first look at their coefficients.

4. Coefficients of TIRK methods

In a way reminiscent of the *collocation polynomial* found in classical algebraic collocation techniques, it was shown in [16, Theorem 2.3] under a mild interpolation condition that any functionally fitted method has a corresponding *collocation solution* which is a linear combination of the basis functions. This result applies to TIRK methods as a consequence of the existence and unicity of the interpolation polynomial in the trigonometric case as well (cf., e.g., [14, p. 163]).

We shall now denote $u(t)$ the collocation solution associated with a TIRK method. It satisfies the differential equation at the collocation points, i.e.,

$$u(t_n) = y_n, \quad u'(t_n + c_i h) = f(t_n + c_i h, u(t_n + c_i h)), \quad i = 1, \ldots, s.$$

Similarly to classical collocation results (see, e.g., [22, p. 473] for RKN) we have the following characterization.

Theorem 8. *The coefficients $\boldsymbol{A} = (a_{ij})_{i,j=1}^s$ and $\boldsymbol{b} = (b_1, \ldots, b_s)^{\mathrm{T}}$ of an s-stage TIRK method are defined by*

$$a_{ij} := \alpha_j(c_i), \quad b_i := \alpha_i(1), \quad \alpha_i(x) = \int_0^x L_i^*(t)\,\mathrm{d}t, \tag{6}$$

where

$$L_i^*(x) = \begin{cases} L_i(x) & \text{if } s = 2r+1, \\ L_i(x) \dfrac{\sum_{j=0}^r P(x_j) \dfrac{\sin(((x - x_j)/2)v)}{\sin(((c_i - x_j)/2)v)}}{\sum_{j=0}^r P(x_j)}, \quad x_j = \dfrac{2j\pi}{(r+1)v} & \text{if } s = 2r, \end{cases} \tag{7}$$

with

$$L_i(x) = \prod_{\substack{k=1 \\ k \neq i}}^s \frac{\sin(((x - c_k)/2)v)}{\sin(((c_i - c_k)/2)v)}, \quad P(x) = \prod_{k=1}^s \sin\left(\frac{x - c_k}{2} v\right). \tag{8}$$

Proof. Denote $t_{n,i} = t_n + c_i h$ for $i = 1, \ldots, s$. For the case $s = 2r + 1$, since $u(t)$ is a linear combination of the basis functions, we can write $u(t_n + xh) = \alpha_0 + \beta_0 x + \sum_{k=1}^r a_k \cos(kvx) + b_k \sin(kvx)$. This implies that $u'(t_n + xh)$ is a trigonometric polynomial of degree r. Since it naturally interpolates the points $(t_{n,i}, u'(t_{n,i}))_{i=1}^s$, applying the interpolation theorem with these points, we have

$$u'(t_n + hx) = \sum_{i=1}^s u'(t_{n,i}) L_i(x). \tag{9}$$

For the case $s = 2r$, we have the form $u(t_n + xh) = a_0 + \sum_{k=1}^r a_k \cos(kvx) + b_k \sin(kvx)$. This implies that

$$u'(t_n + hx) = \sum_{k=1}^r (a_k' \cos(kvx) + b_k' \sin(kvx)) = \sum_{k=1}^r (c_k \mathrm{e}^{\mathrm{i}kvx} + d_k \mathrm{e}^{-\mathrm{i}kvx})$$

with a'_k, b'_k, c_k, d_k defined appropriately. Observe that if we set $v\alpha = \pm\frac{2\pi}{r+1}$, then $\sum_{j=0}^{r} \mathrm{e}^{\mathrm{i}kvj\alpha} = (\mathrm{e}^{\mathrm{i}k(r+1)v\alpha} - 1)/(\mathrm{e}^{\mathrm{i}kv\alpha} - 1) = 0$, $\forall k = 1, \ldots, r$. Therefore, if we choose $x_j = 2j\pi/v(r+1) = j\alpha/v$, $j = 0, \ldots, r$, we have the identity

$$\sum_{j=0}^{r} u'(t_n + x_j h) = \sum_{k=1}^{r} \left[c_k \sum_{j=0}^{r} \mathrm{e}^{\mathrm{i}kvx_j} + d_k \sum_{j=0}^{r} \mathrm{e}^{-\mathrm{i}kvx_j} \right] = 0. \tag{10}$$

Now, for a fixed $0 \leqslant j \leqslant r$, defining the extra node $t_{n,s+1} = t_n + x_j h$, and applying the interpolation theorem at $(t_{n,i})_{i=1}^{s+1}$, we have

$$u'(t_n + xh) = \sum_{i=1}^{s} u'(t_{n,i}) L_i(x) \frac{\sin(((x - x_j)/2)v)}{\sin(((c_i - x_j)/2)v)} + u'(t_n + x_j h) \frac{P(x)}{P(x_j)}.$$

This implies that

$$u'(t_n + xh) P(x_j) = \sum_{i=1}^{s} u'(t_{n,i}) L_i(x) \frac{\sin(((x - x_j)/2)v)}{\sin(((c_i - x_j)/2)v)} P(x_j) + u'(t_n + x_j h) P(x).$$

Running $j = 0, \ldots, r$ and summing both sides while taking into account (10), we get

$$u'(t_n + xh) \sum_{j=0}^{r} P(x_j) = \sum_{i=1}^{s} u'(t_{n,i}) L_i(x) \sum_{j=0}^{r} P(x_j) \frac{\sin(((x - x_j)/2)v)}{\sin(((c_i - x_j)/2)v)}.$$

From this equation and (9), and the combined notation of $L_i^*(x)$ in (7), it follows that we can use the following unified result for both the case $s = 2r$ and the case $s = 2r + 1$:

$$u'(t_n + xh) = \sum_{i=1}^{s} L_i^*(x) u'(t_{n,i}).$$

Therefore,

$$u(t_n + xh) = u(t_n) + h \sum_{i=1}^{s} \alpha_i(x) u'(t_{n,i}).$$

And this allows us to recover the coefficients (6) as the classical case. □

5. Stability analysis of TIRK methods

We will reveal the stability function of TIRK methods in general. We will see that it involves several parameters that make its appreciation not immediate. Consequently, we start this section by first considering the example of a two-stage method that we study in detail to illustrate the issues and define the notation. It also allows us to highlight the connections with similar topics in the literature.

5.1. Two-stage TIRK method (TIRK2)

Consider the case where $r = 1$ and $s = 2r = 2$, it can be shown that the coefficients of TIRK2 are given by the Butcher-tableau (cf. [21])

$$\begin{array}{c|cc} c_1 & \dfrac{\cos(c_2\nu)-\cos[(c_2-c_1)\nu]}{\nu\sin[(c_1-c_2)\nu]} & \dfrac{1-\cos(c_1\nu)}{\nu\sin[(c_1-c_2)\nu]} \\ c_2 & \dfrac{\cos(c_2\nu)-1}{\nu\sin[(c_1-c_2)\nu]} & \dfrac{\cos[(c_2-c_1)\nu]-\cos(c_1\nu)}{\nu\sin[(c_1-c_2)\nu]} \\ \hline & \dfrac{\cos[(1-c_1)\nu]-\cos(c_1\nu)}{\nu\sin[(c_1-c_2)\nu]} & \dfrac{\cos(c_2\nu)-\cos[(1-c_2)\nu]}{\nu\sin[(c_1-c_2)\nu]} \end{array}, \quad \nu \equiv \omega h. \tag{11}$$

Such closed-formed expressions tend to be cumbersome in general. They can be obtained from Theorem 8 or by applying Cramer rules to the linear system resulting from (2), as done in [21] from a different perspective. In fact, $2r$-stage TIRK methods can be viewed as methods constructed to maximise the *trigonometric order* first defined in Gautschi [10] and pursued in [21]. Any $2r$-stage TIRK method is a method in [21] with a trigonometric order r.

As apparent from (11), the coefficients need special care when v is small. Recall that the method approaches a constant coefficient method when $h \to 0$. In practice, we assume $v = \omega h > 0$ and switch to a Radau-type method when $v \to 0$. From general results seen earlier, the stage order is 2. Superconvergence is obtained by choosing (c_1, c_2) as Gauss points $c_1 = (3-\sqrt{3})/6$, $c_2 = (3+\sqrt{3})/6$, yielding a method with an order of accuracy of 4. Notice in general that if we choose (c_1, c_2) such that $c_1 + c_2 = 1$, we end up with $b_1 = b_2$. Our study will give a special attention to TIRK methods that use symmetric points, i.e., when $(c_i)_{i=1}^{2r}$ are symmetric around $\frac{1}{2}$, meaning $c_i + c_{2r+1-i} = 1$.

Applying the Runge–Kutta method (11) to the Dahlquist test equation

$$y' = \lambda y$$

we get the iteration scheme

$$y_{n+1} = R(v, \lambda h) y_n,$$

where

$$R(v,z) = 1 + z\boldsymbol{b}^{\mathrm{T}}(v)(I - z\boldsymbol{A}(v))^{-1}\boldsymbol{e} = \frac{\det[I - z\boldsymbol{A}(v) + z\boldsymbol{e}\boldsymbol{b}^{\mathrm{T}}(v)]}{\det[I - z\boldsymbol{A}(v)]}$$

is the well-known stability function (see [1, p. 86]), which in our case depends on v as well.

As first pointed out by Coleman and Ixaru [5], such a dependency entails recasting classical definitions to suit the variable coefficient context in a practically useful way while still remaining consistent with the spirit of the original definitions. Coleman and Ixaru [5] and subsequently Carpentieri and Paternoster [3] viewed methods such as (11) as a *family* of methods[1] and defined the family as stable if *all* the methods in the family were stable. We take a slightly different view by considering (11) as a single method (with ω choosen in advance) and we then define it as A-stable if it can withstand any Dahlquist test equation, i.e., whatever the value of λ in the negative half-plane.

Definition 9 (*A-stable method*). A TIRK method with variable coefficients $(\boldsymbol{c}, \boldsymbol{b}(v), \boldsymbol{A}(v))$, with the stability function $R(v,z)$ above, is said to be A-stable at $v = v_0 > 0$ if $|R(v_0, z)| \leqslant 1$, $\forall z \in \mathbb{C}^-$.

Remark 10. It is clear that a TIRK method is stable if it is A-stable at small enough values of v. It is recommended to choose $\boldsymbol{c}$ so that the algebraic method is A-stable. This will ensure that the TIRK method is A-stable in the limit as $v \to 0$ because the stability function $R(v,z) = \det[I - z\boldsymbol{A}(v) + z\boldsymbol{e}\boldsymbol{b}(v)^{\mathrm{T}}]/\det[I - z\boldsymbol{A}(v)]$ converges to the conventional

[1] Our notation is inverted from that in [5,3] where they instead use ω as the frequency of their harmonic oscillator test equation $y'' = -\omega^2 y$, while the main parameter is $\theta = kh$, with k being the fitted frequency meant to be choosen to select a method in the family. Our v here plays the role of their θ but our test equation is the Dahlquist test equation involving λ.

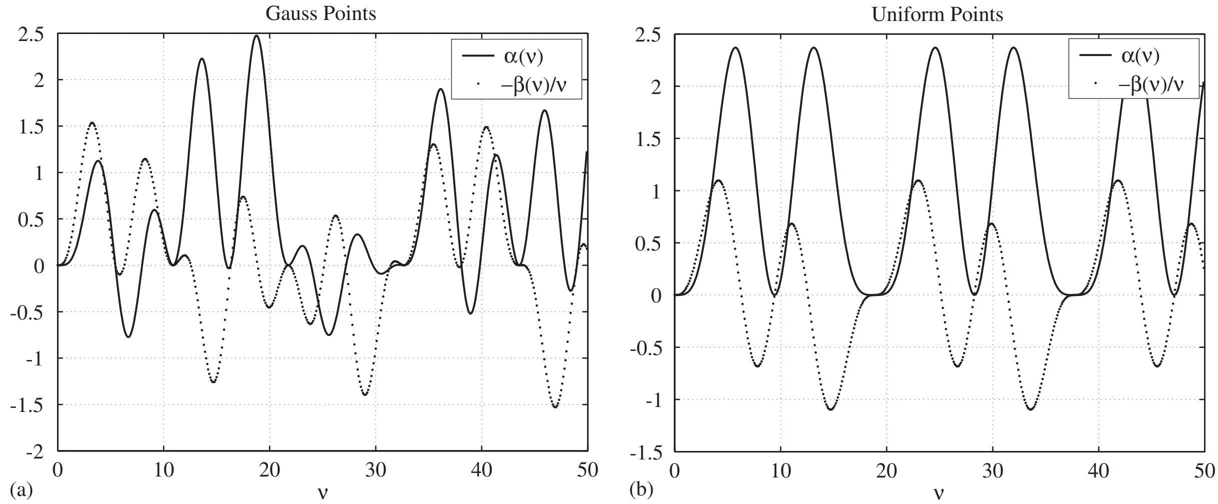

Fig. 1. Plots of $\alpha(v)$ and $-\beta(v)/v$ using Gauss points and uniform points. TIRK2 is A-stable when both $\alpha(v)>0$ and $-\beta(v)/v>0$. It can be seen that satisfactory values of v occur in intermittent intervals.

function due to the convergence of $\boldsymbol{A}(v)$ and $\boldsymbol{b}(v)$. This convergence also means that any TIRK method is zero-stable since as $v\to 0$, we get the conventional function which as we already know, is always zero-stable.

Consider now the problem of finding the subset $S\subset(0,+\infty)$ such that TIRK2 is A-stable for all $v\in S$. From (11), direct calculation shows that its stability function is

$$R(v,z)=\frac{v^2\alpha_4^2-v\alpha_4(\alpha_2-\alpha_1)z+[(\alpha_3-1)(\alpha_1+\alpha_2)+\alpha_4^2]z^2}{v^2\alpha_4^2+v\alpha_4(\alpha_2-\alpha_1)z+[(\alpha_3-1)(\alpha_1+\alpha_2)+\alpha_4^2]z^2}\equiv\frac{p(-z)}{p(z)}, \tag{12}$$

where

$$\alpha_1=\cos(c_1v),\quad \alpha_2=\cos(c_2v),\quad \alpha_3=\cos[(c_2-c_1)v],\quad \alpha_4=\sin[(c_2-c_1)v].$$

It is clear that $|R(v,iy)|=1,\ \forall y\in\mathbb{R}$. Hence, by the maximum principle, the method will be A-stable if $R(v,z)$ has no poles in the left plane (see [12, p. 88]), i.e., if the denominator polynomial $p(z)$ in (12) has no roots in the left plane. Writing

$$p(z)=\alpha z^2+\beta z+\gamma,$$

where

$$\alpha\equiv\alpha(v)=(\alpha_3-1)(\alpha_1+\alpha_2)+\alpha_4^2,\quad \beta\equiv\beta(v)=v\alpha_4(\alpha_2-\alpha_1),\quad \gamma\equiv\gamma(v)=v^2\alpha_4^2$$

we see that $p(z)$ has no roots in $\mathbb{C}^-$ if $\alpha\gamma>0$ and $\beta/\alpha<0$. Since $\gamma>0$ by construction, we just need to have $\alpha>0$ and $\beta<0$.

Using MATLAB with (c_1,c_2) being the two Gauss points $(3-\sqrt{3})/6$, $(3+\sqrt{3})/6$, we see that there are indeed intermittent intervals for v satisfying the conditions, though they vary in an unpredictable way (see Fig. 1a).

If we choose (c_1,c_2) such that $(c_1+c_2)/(c_2-c_1)=1/(c_2-c_1)$ is an integer value, then both $\alpha(v)$ and $-\beta(v)/v$ become periodic functions as illustrated in Fig. 1b using the uniform points $c_1=\frac{1}{3}$ and $c_2=\frac{2}{3}$. It can be shown with these points that the solutions for $\alpha(v)>0$ and $-\beta(v)/v>0$ are $6k\pi<v<6k\pi+2\pi$; or $6k\pi+3\pi<v<6k\pi+4\pi$, $\forall k=0,1,\ldots$. Should we pick such a v and construct the corresponding RK method $(\boldsymbol{c},\boldsymbol{b}(v),\boldsymbol{A}(v))$, it will be A-stable. More generally, it can be shown analytically that any two-stage TIRK method with symmetric collocation points is A-stable for all $v\in(0,\pi]$. The symmetry is only a sufficient condition and other A-stable methods exist. Having suitable values of v in a large interval means that the methods can cope well with applications where the frequency is not known exactly. It also allows changing the stepsize during the integration of stiff systems, without worrying about stability.

As another interesting by-product, it can be shown with the same technique that any arbitrary pair of symmetric collocation parameters (c_1, c_2) leads to an A-stable algebraic RK method.

5.2. Stability function of $2r$-stage TIRK methods

We turn once more to the collocation solution $u(x)$ which in this case is a trigonometric polynomial of degree r that satisfies the differential equation at the collocation points, i.e.,

$$u(x_0) = y_0, \quad u'(x_0 + c_i h) = f(x_0 + c_i h, u(x_0 + c_i h)), \quad i = 1, \ldots, s. \tag{13}$$

We now set without loss of generality $x_0 = 0$, $x_1 = 1$, $h = 1$, $y_0 = 1$, $\lambda = z$, and use a similar technique as in classical methods (see [12, p. 48]) to establish the following result.

Theorem 11. *The stability function of a $2r$-stage TIRK method is*

$$R(v, z) = \frac{-a_0 \dfrac{1}{z} + \sum_{k=1}^{r} a_k \dfrac{-z\cos(kv) + kv\sin(kv)}{z^2 + (kv)^2} + \sum_{k=1}^{r} b_k \dfrac{-z\sin(kv) - kv\cos(kv)}{z^2 + (kv)^2}}{-a_0 \dfrac{1}{z} + \sum_{k=1}^{r} a_k \dfrac{-z}{z^2 + (kv)^2} + \sum_{k=1}^{r} b_k \dfrac{-kv}{z^2 + (kv)^2}}, \tag{14}$$

where

$$\begin{aligned} a_0 &= \frac{v}{2\pi} \int_0^\theta M(v, \xi)\, \mathrm{d}\xi, \quad \theta \equiv \frac{2\pi}{v}, \\ a_k &= \frac{v}{\pi} \int_0^\theta M(v, \xi) \cos(kv\xi)\, \mathrm{d}\xi, \quad b_k = \frac{v}{\pi} \int_0^\theta M(v, \xi) \sin(kv\xi)\, \mathrm{d}\xi, \quad k = 1, \ldots, r. \end{aligned} \tag{15}$$

are the coefficients of the Fourier series of the trigonometric function

$$M(v, x) = \prod_{i=1}^{s} \sin \frac{xv - c_i v}{2}.$$

Proof. Since $u'(x) - zu(x)$ is a trigonometric polynomial of degree r that vanishes at the collocation points, there is a constant K such that

$$u'(x) - zu(x) = KM(v, x), \quad u(x_0) = y_0 = 1.$$

This inhomogeneous equation can be solved by the variation of constant formula to obtain

$$u(x) = \mathrm{e}^{zx} \left(K \int_0^x \mathrm{e}^{-\xi z} M(v, \xi)\, \mathrm{d}\xi + 1 \right). \tag{16}$$

From the fact that $M(v, x)$ is a trigonometric polynomial of degree $r = s/2$, it can be represented in Fourier series form as

$$M(v, x) = a_0 + \sum_{k=1}^{r} (a_k \cos(kvx) + b_k \sin(kvx)), \tag{17}$$

where the coefficients in the series are defined by (15). Using the following intermediate results:

$$\int_0^x \mathrm{e}^{-\xi z}\,\mathrm{d}\xi = -\frac{1}{z}\mathrm{e}^{-xz} + \frac{1}{z},$$

$$\int_0^x \mathrm{e}^{-\xi z}\cos(kv\xi)\,\mathrm{d}\xi = \frac{z}{z^2+(kv)^2} + \frac{-z\cos(kvx)+kv\sin(kvx)}{z^2+(kv)^2}\mathrm{e}^{-zx},$$

$$\int_0^x \mathrm{e}^{-\xi z}\sin(kv\xi)\,\mathrm{d}\xi = \frac{kv}{z^2+(kv)^2} + \frac{-z\sin(kvx)-kv\cos(kvx)}{z^2+(kv)^2}\mathrm{e}^{-zx},$$

we obtain

$$\begin{aligned}\int_0^x \mathrm{e}^{-\xi z}M(v,\xi)\,\mathrm{d}\xi &= a_0\int_0^x \mathrm{e}^{-\xi z}\,\mathrm{d}\xi + \sum_{k=1}^{r}\int_0^x \mathrm{e}^{-\xi z}(a_k\cos(kv\xi)+b_k\sin(kv\xi))\,\mathrm{d}\xi \\ &= \tilde{a}_0 + \mathrm{e}^{-zx}\left(\tilde{c} + \sum_{k=1}^{r}(\tilde{a}_k\cos(kvx)+\tilde{b}_k\sin(kvx))\right),\end{aligned}$$

where

$$\tilde{a}_0 = \frac{a_0}{z} + \sum_{k=1}^{r}\frac{a_k z + b_k kv}{z^2+(kv)^2}, \quad \tilde{c} = -\frac{a_0}{z},$$

$$\tilde{a}_k = -\frac{za_k + kvb_k}{z^2+(kv)^2}, \quad \tilde{b}_k = \frac{kva_k - zb_k}{z^2+(kv)^2}.$$

It follows from (16) that

$$u(x) = \mathrm{e}^{zx}(K\tilde{a}_0+1) + K\left(\tilde{c} + \sum_{k=1}^{r}(\tilde{a}_k\cos(kvx)+\tilde{b}_k\sin(kvx))\right).$$

Since $u(x)$ is a trigonometric polynomial, the first term must vanish, i.e.,

$$K = -\frac{1}{\tilde{a}_0} = -1\bigg/\left[\frac{a_0}{z} + \sum_{k=1}^{r}\frac{a_k z + b_k kv}{z^2+(kv)^2}\right],$$

and evaluating $u(1)$ gives the stability function

$$R(v,z) = K\left(\tilde{c} + \sum_{k=1}^{r}(\tilde{a}_k\cos(kv)+\tilde{b}_k\sin(kv))\right)$$

which expands into (14). □

5.2.1. Stability function of two-stage TIRK, again

It is not immediately apparent how to further simplify the general stability function (14) to avoid Fourier coefficients. We previously obtained the much simpler expression (12) for the two-stage method. Intriguingly, the two results bear little resemblance. We show here that they indeed coincide (this was the motivation of our direct derivation earlier). When $s=2$ we have

$$M(v,x) = \prod_{i=1}^{2}\sin\frac{(x-c_i)v}{2} = a_0 + a_1\cos(vx) + b_1\sin(vx)$$

where

$$a_0 = \frac{1}{2}\cos\frac{(c_2-c_1)v}{2}, \quad a_1 = -\frac{1}{2}\cos\frac{(c_1+c_2)v}{2}, \quad b_1 = -\frac{1}{2}\sin\frac{(c_1+c_2)v}{2}.$$

It follows from (14) that

$$R(v,z)=\frac{z^2(a_0+a_1\cos v+b_1\sin v)+zv(-a_1\sin v+b_1\cos v)+v^2a_0}{z^2(a_0+a_1)+zvb_1+v^2a_0}. \tag{18}$$

If we choose (c_1, c_2) such that $c_1+c_2=1$, some trigonometric manipulations lead to

$$R(v,z)=\frac{z^2(a_0+a_1)-zvb_1+a_0v^2}{z^2(a_0+a_1)+zvb_1+a_0v^2}.$$

It is easy to check that

$$\frac{(\alpha_3-1)(\alpha_1+\alpha_2)+\alpha_4^2}{a_0+a_1}=\frac{\alpha_2-\alpha_1}{b_1}=\frac{\alpha_4^2}{a_0}=4\sin\frac{(c_2-c_1)v}{2}\sin[(c_2-c_1)v],$$

where the α_i are defined in (12). Hence we recover the formula obtained earlier in (12).

Remark 12. For the two-stage method, notice that the stability function (18) can be put in the form

$$R(v,z)=\frac{z^2M(v,1)+zM'(v,1)+\kappa}{z^2M(v,0)+zM'(v,0)+\kappa},$$

where

$$\kappa=v^2a_0=M''(v,1)-M(v,1)=M''(v,0)-M(v,0).$$

This representation matches that of the stability function of algebraic RK methods. But it is not retained when $r>1$. In fact in the algebraic RK context, one can take the derivative of the equation $u'(x)-zu(x)=KM(v,x)$ s times to get the stability function. But this technique is ineffective in the trigonometric context.

5.2.2. Stability function of four-stage TIRK

We consider now the case where $r=2$ and $s=2r=4$. We study the stability function in detail since this method can attain a high order of 8 and be of interest to implementors. Assuming once more symmetric collocation points, we obtain

$$M(v,x)=\prod_{i=1}^{4}\sin\left(\tfrac{x-c_i}{2}\right)v=a_0+a_1\cos(xv)+b_1\sin(xv)+a_2\cos(2xv)+b_2\sin(2xv), \tag{19}$$

where

$$a_0=\frac{ab}{4}+\frac{1}{8},\quad a_1=-\frac{a+b}{4}\cos\frac{v}{2},\quad a_2=\frac{1}{8}\cos v,\quad a=\cos\frac{(c_4-c_1)v}{2},$$

$$b_1=-\frac{a+b}{4}\sin\frac{v}{2},\quad b_2=\frac{1}{8}\sin v,\quad b=\cos\frac{(c_3-c_2)v}{2}.$$

Denote $P(z)$ the denominator of the stability function (14). For $r=2$, it can be expressed as

$$P(z)=\frac{z^4(a_0+a_1+a_2)+z^3v(b_1+2b_2)+z^2v^2(5a_0+4a_1+a_2)+zv^3(4b_1+2b_2)+4v^4a_0}{z(z^2+v^2)(z^2+4v^2)}$$

We wish to establish the conditions under which it has no roots in the left plane. We use the Routh–Hurwitz criteria (see [11, p. 85]) which state that the roots of a normalized quartic polynomial $Q(z)=z^4+pz^3+qz^2+rz+s$ lie in the negative half complex plane $\mathbb{C}^-$ if and only if $p>0$, $pq-r>0$, $(pq-r)r-p^2s>0$, and $s>0$. To apply the criteria in our context, we consider $P(-z)$ instead and study the following normalized polynomial

$$Q(z)=\frac{P(-z)(-z)(z^2+v^2)(z^2+4v^2)}{a_0+a_1+a_2}=z^4+pz^3+qz^2+rz+s$$

where

$$p \equiv p(v) = -\frac{v(b_1 + 2b_2)}{a_0 + a_1 + a_2}, \quad r \equiv r(v) = -\frac{v^3(4b_1 + 2b_2)}{a_0 + a_1 + a_2},$$

$$q \equiv q(v) = \frac{v^2(5a_0 + 4a_1 + a_2)}{a_0 + a_1 + a_2}, \quad s \equiv s(v) = \frac{4v^4 a_0}{a_0 + a_1 + a_2}.$$

From (19) we have

$$a_0 + a_1 + a_2 = M(v, 0) = \prod_{i=1}^{4} \sin\left(\frac{c_i v}{2}\right) > 0 \quad \text{if } 0 < c_i v < 2\pi.$$

Furthermore, we can show that

$$b_1 + 2b_2 = -\frac{1}{2}\left(\sin\frac{c_4 v}{2}\sin\frac{c_1 v}{2} + \sin\frac{c_3 v}{2}\sin\frac{c_2 v}{2}\right)\sin\frac{v}{2} < 0 \quad \text{if } 0 < c_i v, \frac{v}{2} < \pi.$$

These show that $s > 0$ and $p > 0$ if $0 < c_i v, v/2 < \pi$. Hence we only need to study the remaining two conditions $pq - r > 0$ and $(pq - r)r - p^2 s > 0$. Again, by using MATLAB we see that there are intermittent intervals for v in which these conditions are met. In particular, we notice that values of $v \in (0, \pi]$ are satisfactory.

5.2.3. Stability of $2r$*-stage TIRK methods with symmetric points*

We have seen so far that there are interesting properties when the two-stage and four-stage TIRK methods are constructed with symmetric collocation points. This section builds on these observations to provide some general results. The starting point is the stability function.

Theorem 13. *Assume that* $(c_i)_{i=1}^{2r}$ *are symmetric around* $\frac{1}{2}$, *i.e.,* $c_i + c_{2r+1-i} = 1$ *for* $i = 1, \ldots, r$, *then the stability function* (14) *in the case of a* $2r$*-stage TIRK method with symmetric points can be simplified as*

$$R(v, z) = \frac{-a_0\frac{1}{z} + \sum_{k=1}^{r} a_k \frac{-z}{z^2 + (kv)^2} - \sum_{k=1}^{r} b_k \frac{-kv}{z^2 + (kv)^2}}{-a_0\frac{1}{z} + \sum_{k=1}^{r} a_k \frac{-z}{z^2 + (kv)^2} + \sum_{k=1}^{r} b_k \frac{-kv}{z^2 + (kv)^2}} = 1/R(v, -z). \tag{20}$$

Proof. To prove this, we first prove the identities

$$a_k = a_k \cos(kv) + b_k \sin(kv), \quad b_k = a_k \sin(kv) - b_k \cos(kv), \quad k = 1, \ldots, r.$$

The assumption $c_i = 1 - c_{2r+1-i}$ gives

$$\sin\frac{(x - c_i)v}{2} = -\sin\frac{(1 - x - c_{2r+1-i})v}{2}.$$

Hence

$$M(v, x) = \prod_{i=1}^{2r} \sin\frac{(x - c_i)v}{2} = (-1)^{2r} \prod_{i=1}^{2r} \sin\frac{(1 - x - c_{2r+1-i})v}{2} = M(v, 1 - x).$$

From the definitions of a_k and b_k in (15), we get

$$\begin{aligned} a_k \cos(kv) + b_k \sin(kv) &= \frac{v}{\pi}\int_0^{\theta} M(v, \xi)\cos(kv(1 - \xi))\,\mathrm{d}\xi \\ &= \frac{v}{\pi}\int_{1-\theta}^{1} M(v, 1 - \xi)\cos(kv\xi)\,\mathrm{d}\xi, \\ &= \frac{v}{\pi}\int_{1-\theta}^{1} M(v, \xi)\cos(kv\xi)\,\mathrm{d}\xi. \end{aligned}$$

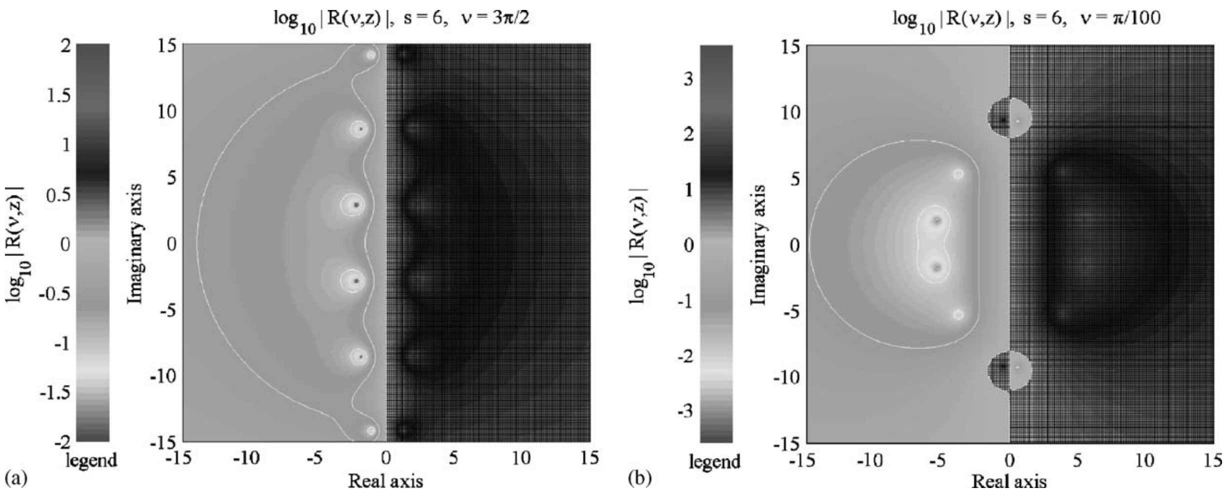

Fig. 2. Plots of $\log_{10}|R(v,z)|$ in the complex plane using a six-stage method with uniform and symmetric points $\boldsymbol{c}=(\frac{1}{7},\frac{2}{7},\frac{3}{7},\frac{4}{7},\frac{5}{7},\frac{6}{7})^{\mathrm{T}}$ at $v=3\pi/2$ in (a) and $v=\pi/100$ in (b). From the colorbar legend, $R(v,z)$ in (a) has no poles in $\mathbb{C}^-$ because $\mathbb{C}^-$ is entirely gray. Plot (b) shows two disks where the modulus exceeds 1.

The integrand $M(v,\xi)\cos(kv\xi)$ is a trigonometric polynomial of frequency v, hence it is periodic with period $\theta=2\pi/v$. Recall the property that the integration of a trigonometric polynomial over one period (which is θ here) is constant. Therefore,

$$\frac{v}{\pi}\int_{1-\theta}^{1} M(v,\xi)\cos(kv\xi)\,\mathrm{d}\xi=\frac{v}{\pi}\int_{0}^{\theta} M(v,\xi)\cos(kv\xi)\,\mathrm{d}\xi=a_k.$$

The identity involving b_k can be proved similarly. Using these identities in (14) we get (20). □

In general, therefore, the stability function is simplified to a much nicer form when using symmetric collocation points. From there it is easy to verify that $|R(v,iy)|=1,\ \forall y\in\mathbb{R}$. Consequently, by the maximum principle, a method will be A-stable if it is constructed with a parameter v such that $R(v,z)$ has no pole in the left half complex plane. We saw earlier that the two-stage and four-stage methods were A-stable when constructed with $v\in(0,\pi]$. We found in experiments that for $r=3$ the 6-stage method with uniform symmetric collocation points $\boldsymbol{c}=(\frac{1}{7},\frac{2}{7},\frac{3}{7},\frac{4}{7},\frac{5}{7},\frac{6}{7})^{\mathrm{T}}$ is not A-stable with some, even small, $v\in(0,\pi]$ such as $v=\pi/10$ and $v=\pi/100$. Further checking showed that this $\boldsymbol{c}$ does not lead to an A-stable conventional method. Therefore, it is not a suitable choice as we indicated in Remark 10. We note however that it is A-stable at $v=3\pi/2$. See Fig. 2 which plots the log of the modulus of $R(v,z)$ in the two cases $v=\pi/100$ and $v=3\pi/2$.

5.3. *Stability function of* $(2r+1)$*-stage TIRK methods*

As in Section 5.2, we use the collocation function $u(x)$ that uniquely characterizes any given $(2r+1)$-stage TIRK method. Its form here is

$$u(x)=\alpha_0 x+\beta_0+\sum_{k=1}^{r}(\alpha_k\cos(kvx)+\beta_k\sin(kvx)),$$

where $\alpha_k,\beta_k,k=0,\ldots,r$, are coefficients that only depend on $(c_i)_{i=1}^{2r+1}$, v and $\lambda=z$. This function has the special interpolation property that $u'(x)-zu(x)$ vanishes at the collocation points. As in the previous case, $u'(x)-zu(x)$ also has the same form as $u(x)$, which we write for convenience of notation as

$$u'(x)-zu(x)=K(x-M(v,x))$$

where K is a constant and $M(v, x)$ is a trigonometric polynomial of degree r and frequency v. Given that $u'(c_i)-zu(c_i)=0$ for $i = 1, \dots, s$, we have $M(v, c_i) - c_i = 0$, and so M can be represented using the Lagrange interpolation formula

$$M(v, x) = \sum_{i=1}^{s} c_i L_i(v, x), \quad L_i(v, x) = \prod_{\substack{j=1\\ j\neq i}}^{s} \frac{\sin(((x - c_j)/2)v)}{\sin(((c_i - c_j)/2)v)}.$$

Hence

$$u'(x) - zu(x) = K\left(x - \sum_{i=1}^{s} c_i L_i(v, x)\right)$$

and using a similar approach as in Theorem 11, we can show the following result.

Theorem 14. *The stability function of a* $(2r + 1)$*-stage TIRK method is*

$$R(v, z) = \frac{-\dfrac{1}{z} + a_0\dfrac{1}{z} - \dfrac{1}{z^2} + \sum_{k=1}^{r} a_k \dfrac{z\cos(kv) - kv\sin(kv)}{z^2 + (kv)^2} + \sum_{k=1}^{r} b_k \dfrac{z\sin(kv) + kv\cos(kv)}{z^2 + (kv)^2}}{a_0\dfrac{1}{z} - \dfrac{1}{z^2} + \sum_{k=1}^{r} a_k \dfrac{z}{z^2 + (kv)^2} + \sum_{k=1}^{r} b_k \dfrac{kv}{z^2 + (kv)^2}}.$$

in which the coefficients a_k *and* b_k *are those of the Fourier series expansion of* $M(v, x) = \sum_{i=1}^{s} c_i L_i(v, x) = a_0 + \sum_{k=1}^{r} (a_k \cos(kvx) + b_k \sin(kvx))$.

5.3.1. Stability of $(2r + 1)$*-stage methods with symmetric collocation points*

Since $s = 2r + 1$ is odd, we define symmetric collocation points here as $c_i + c_{s+1-i} = 1$, for $i = 1, \dots, r$, and $c_{r+1} = \frac{1}{2} = 1 - c_{r+1}$. Now, replacing $c_i := 1 - c_{s+1-i}$ in each Lagrange factor above, we can easily verify that

$$c_i L_i(v, x) = (1 - c_{s+1-i}) L_{s+1-i}(v, 1 - x).$$

It follows therefore that

$$M(v, x) = \sum_{i=1}^{s} c_i L_i(v, x) = \sum_{i=1}^{s} L_i(v, 1 - x) - \sum_{i=1}^{s} c_i L_i(v, 1 - x) = 1 - M(v, 1 - x).$$

From there, similarly to the identities shown in the proof of Theorem 13 for the even case, we can show in the present odd case that

$$a_0 = \tfrac{1}{2}, \quad -a_k = a_k \cos(kv) + b_k \sin(kv), \quad b_k = b_k \cos(kv) - a_k \sin(kv).$$

And using these identities in Theorem 14, we obtain the following result.

Theorem 15. *The stability function of a* $(2r + 1)$*-stage TIRK method with symmetric collocation points is*

$$R(v, z) = \frac{-\dfrac{1}{z^2} - \dfrac{1}{2z} - \sum_{k=1}^{r} a_k \dfrac{z}{z^2 + (kv)^2} + \sum_{k=1}^{r} b_k \dfrac{kv}{z^2 + (kv)^2}}{-\dfrac{1}{z^2} + \dfrac{1}{2z} + \sum_{k=1}^{r} a_k \dfrac{z}{z^2 + (kv)^2} + \sum_{k=1}^{r} b_k \dfrac{kv}{z^2 + (kv)^2}} = 1/R(v, -z) \tag{21}$$

in which the coefficients a_k *and* b_k *are those of the Fourier series expansion of* $M(v, x) = \sum_{i}^{s} c_i L_i(v, x) = a_0 + \sum_{k=1}^{r} (a_k \cos(kvx) + b_k \sin(kvx))$.

From there it is easy to verify that $|R(v, \mathrm{i}y)| = 1$, $\forall y \in \mathbb{R}$. Again, by the maximum principle, a method will be A-stable if it is constructed with a parameter v such that $R(v, z)$ has no pole in the left half complex plane.

As it can be seen, the stability function is not easy to calculate explicitly in general. The Lagrange factors make the case $s = 2r + 1$ even more cumbersome than the case $s = 2r$.

5.3.2. Three-stage TIRK method

For the particular case of the three-stage TIRK method, applying Theorem 8, we obtain the coefficients

$$\begin{array}{c|c} \boldsymbol{c} & \boldsymbol{A} \\ \hline & \boldsymbol{b}^{\mathrm{T}} \end{array}, \quad \boldsymbol{c} = (c_1, c_2, c_3)^{\mathrm{T}}, \quad \boldsymbol{A} = (a_{ij})_{i,j=1}^{3}, \quad \boldsymbol{b} = (b_1, b_2, b_3)^{\mathrm{T}},$$

where

$$a_{ij} = \alpha_j(c_i), \quad b_i = \alpha_i(1), \quad i, j = 1, 2, 3, \tag{22}$$

with

$$\delta_1 = \frac{c_2 - c_3}{2}, \quad \delta_2 = \frac{c_3 - c_1}{2}, \quad \delta_3 = \frac{c_1 - c_2}{2},$$

$$\alpha_1(x) = \frac{-xv\cos(\delta_1 v) + 2\sin((x/2)v)\cos(((c_2 + c_3 - x)/2)v)}{2v\sin(\delta_2 v)\sin(\delta_3 v)},$$

$$\alpha_2(x) = \frac{-xv\cos(\delta_2 v) + 2\sin((x/2)v)\cos(((c_3 + c_1 - x)/2)v)}{2v\sin(\delta_3 v)\sin(\delta_1 v)},$$

$$\alpha_3(x) = \frac{-xv\cos(\delta_3 v) + 2\sin((x/2)v)\cos(((c_1 + c_2 - x)/2)v)}{2v\sin(\delta_1 v)\sin(\delta_2 v)}.$$

In addition, applying Theorem 14, we obtain the stability function

$$R(v, z) = \frac{a_0\dfrac{1}{z} - \dfrac{1}{z} - \dfrac{1}{z^2} + a_1\dfrac{z\cos v - v\sin v}{z^2 + v^2} + b_1\dfrac{z\sin v + v\cos v}{z^2 + v^2}}{a_0\dfrac{1}{z} - \dfrac{1}{z^2} + a_1\dfrac{z}{z^2 + v^2} + b_1\dfrac{v}{z^2 + v^2}}, \tag{23}$$

where the coefficients

$$-a_0 = \frac{c_1\cos(\delta_1 v)}{2\sin(\delta_2 v)\sin(\delta_3 v)} + \frac{c_2\cos(\delta_2 v)}{2\sin(\delta_3 v)\sin(\delta_1 v)} + \frac{c_3\cos(\delta_3 v)}{2\sin(\delta_1 v)\sin(\delta_2 v)},$$

$$a_1 = \frac{c_1\cos(\frac{c_2+c_3}{2}v)}{2\sin(\delta_2 v)\sin(\delta_3 v)} + \frac{c_2\cos(\frac{c_3+c_1}{2}v)}{2\sin(\delta_3 v)\sin(\delta_1 v)} + \frac{c_3\cos(\frac{c_1+c_2}{2}v)}{2\sin(\delta_1 v)\sin(\delta_2 v)},$$

$$b_1 = \frac{c_1\sin(\frac{c_2+c_3}{2}v)}{2\sin(\delta_2 v)\sin(\delta_3 v)} + \frac{c_2\sin(\frac{c_3+c_1}{2}v)}{2\sin(\delta_3 v)\sin(\delta_1 v)} + \frac{c_3\sin(\frac{c_1+c_2}{2}v)}{2\sin(\delta_1 v)\sin(\delta_2 v)}$$

are obtained by expanding $M(v, x)$ into Fourier series.

5.3.3. Three-stage TIRK method with symmetric points

For the particular case of a three-stage TIRK method with symmetric collocation points $c_1 + c_3 = 1$ and $c_2 = \frac{1}{2}$, the stability function simplifies to (21), and further calculation shows that

$$M(v, x) = \sum_{i=1}^{3} c_i L_i(v, x) = a_0 + a_1\cos(vx) + b_1\sin(vx),$$

where

$$a_0 = \frac{1}{2}, \quad a_1 = -\frac{\frac{1}{2} - c_1}{\sin[(\frac{1}{2} - c_1)v]} \sin\frac{v}{2}, \quad b_1 = \frac{\frac{1}{2} - c_1}{\sin[(\frac{1}{2} - c_1)v]} \cos\frac{v}{2}. \tag{24}$$

To ensure that the resulting method is A-stable, the denominator of the stability function (21) must have no root on the negative half complex plane. Let $P(z)$ denote this denominator. In this particular three-stage case with symmetric points, it can be written as

$$P(z) = \frac{(1+2a_1)z^3 - 2(1-b_1v)z^2 + v^2z - 2v^2}{2z^2(z^2+v^2)}.$$

The Routh–Hurwitz criteria for a normalized cubic polynomial $Q(z) = z^3 + pz^2 + qz + r$ to have all its roots on the negative half complex plane are known to be $p > 0$, $pq - r > 0$, and $r > 0$. Hence, to apply the criteria in our context, we shall consider $P(-z)$ and, for convenience of notation, study the normalized polynomial

$$Q(z) = -P(-z)\frac{2z^2(z^2+v^2)}{1+2a_1} = z^3 + \frac{2(1-b_1v)}{1+2a_1}z^2 + \frac{v^2}{1+2a_1}z + \frac{2v^2}{1+2a_1}.$$

Should $Q(z)$ have all its roots on the left plane, we will conclude that $P(z)$ has all its roots on the right plane. With these preliminaries, we can state the following result.

Theorem 16. *A three-stage TIRK method with symmetric collocation points is A-stable for all* $v \in (0, \min\{\pi/(\frac{1}{2} - c_1), 2\theta\}) \supset (0, 2\pi)$, *where* $\theta \approx 4.4934$ *is the first zero of* $g(x) = x\cos x - \sin x$ *in* $(0, 2\pi]$.

Proof. The Routh–Hurwitz conditions for $Q(z)$ to have all its roots in $\mathbb{C}^-$ are

$$0 < p = \frac{2(1-b_1v)}{1+2a_1}, \quad 0 < pq - r = -\frac{2a_1 + b_1v}{(1+2a_1)^2}, \quad 0 < r = \frac{2v^2}{1+2a_1},$$

where a_1 and b_1 are given by (24). Define $f(x) = \sin x/x$, observe that f is a decreasing function in $(0, 3\pi/2)$. Let $\delta = \frac{1}{2} - c_1$ then $0 < \delta < \frac{1}{2}$. The assumption $v \in (0, \min\{\pi/(\frac{1}{2} - c_1), 2\theta\})$ amounts to $0 < \delta v < \pi$ and $0 < v/2 < \theta$, therefore

$$0 < \delta v < \frac{v}{2} < \theta < \frac{3\pi}{2}.$$

This implies that $f(\delta v) > f(v/2) > 0$. Hence,

$$1 + 2a_1 = \frac{f(\delta v) - f(v/2)}{f(\delta v)} > 0.$$

This shows that the condition $r > 0$ is satisfied and that we only need to study the sign of the numerators of p and $pq - r$. For p, we have

$$1 - b_1v = \frac{f(\delta v) - \cos(v/2)}{f(\delta v)} > \frac{f(v/2) - \cos(v/2)}{f(\delta v)} = -\frac{2g(v/2)}{vf(\delta v)}.$$

For $pq - r$, we have

$$-(2a_1 + b_1v) = 2\frac{(v/2)\cos(v/2) - \sin v/2}{f(\delta v)} = -\frac{2g(v/2)}{f(\delta v)}.$$

Since θ is the first zero of $g(x)$ on the interval $(0, 2\pi]$, we can prove that $g(x) < 0$, $\forall x \in (0, \theta)$. In particular therefore, we have $g(v/2) < 0$. Hence both numerators are positive. □

In our implementation, we actually use collocation points of Radau IIA type, i.e., $\boldsymbol{c} = ((4-\sqrt{6})/10, (4+\sqrt{6})/10, 1)^{\mathrm{T}}$. They are not symmetric. We refer to this method as TIRK3 in our experiments below. Even though we have the expression (23) for its stability function, it is not easy to study its stability region analytically. However, if we use MATLAB to plot the modulus of the stability function, we can also see that it is A-stable for $v \in (0, \pi]$ as was the two-stage and four-stage methods. Experimenting further, we observed that in general, for $s = 2, 3, 4, 5, 6$, the s-stage TIRK method based on common collocation points such as Gauss, Radau IIA, Lobatto, was A-stable for $v \in (0, \pi]$. And if a conventional RK method with symmetric collocation points was A-stable, the corresponding TIRK was also observed to be A-stable with $v \in (0, \pi]$.

Also interesting to note, the stability function of TIRK3, as that of RADAU5, satisfies $R(v, z) < 1$, $\forall z \in \mathbb{C}^-$ and $\rho(R(v, \infty)) = 0$. This property, which resembles L-stability, is critical for a method to work well on very stiff problems. TIRK3 can be regarded as the trigonometric counterpart of RADAU5.

6. Numerical experiments

We only present numerical experiments on stiff periodic problems to show that implicit TIRK methods, with their A-stability property, fit better than both explicit trigonometric and conventional collocation algebraic methods on such problems. For non-stiff periodic problems, explicit trigonometric methods are preferable over implicit trigonometric methods, just like in the taxonomy of explicit conventional methods and implicit conventional methods.

We implemented the three-stage TIRK3 method in MATLAB. As the method is implicit with variable stepsize and variable coefficients, the code updates the coefficients on the fly whenever the stepsize changes (upwards or downwards), e.g., in case of a failure in the Newton scheme when computing the stage values, or a failure or success in satisfying the local truncation error—either of which triggers a new stepsize. We use the explicit formula (22) for the coefficients, but they could also be obtained numerically by solving the linear system resulting from (2) on the fly.

We report numerical comparisons of TIRK3 with a MATLAB implementation of the traditional RADAU5 method. The particular RADAU5 code that we used can be found at [7]. It is a MATLAB port of the original FORTRAN RADAU5 code of Hairer and Wanner [12]. This port retained all the practical aspects that are essential to the competitiveness of RADAU5 (stepsize control, economy of the Jacobian, modified Newton, etc.) as described in detail by Hairer and Wanner [12, p. 128]. Worthy of note is that we were able to re-use this MATLAB RADAU5 implementation for our own TIRK3 implementation. We had to just swap the RADAU5 coefficients with the variable coefficients of TIRK3 and dynamically recompute all the parameters of the code that depend on the coefficients but were implemented under RADAU5 with the assumption that these coefficients were constant. This re-use allowed us to benefit from the subtle tunings and optimizations that have been added to the Radau integrator over the years.

The original RADAU5 code was understandably built with its parameters (coefficients, starting values for the Newton iterations, error estimation) targeted to the algebraic collocation context. We re-used the code while only updating the coefficients and setting trigonometric starting values for the Newton iterations. The resulting code can still be improved to become completely trigonometric, i.e., with trigonometric error estimation and other strategies for controlling the stepsize. Nevertheless, as the experiments will show, on periodic problems with known frequency, it has already turned out to be generally more effective than the original code in all aspects but execution time. There is an overhead in recomputing the coefficients of TIRK3 and the parameters used in solving the linear system each time the stepsize changes. However we expect the cost of these updates to be outweighed by the cost of the function evaluations when the dimension $d \gg 2$ rather than just $d = 2$ as in the tests.

In addition to the classical RADAU5, we include comparisons with EFRK43, an explicit functionally fitted RK method given in [8]. EFRK43 is an embedded pair of order 4(3) based on the method of Zonneveld4(3) (cf. e.g., [11]). We developed a variable stepsize code of EFRK43 following the approach given in [11, pp. 167–169].

Our results include the execution time, but this is shown mostly for fairness and is only indicative because we are in MATLAB. There is a significant overhead from this environment. Besides, the codes are essentially written for correctness and research instead of speed. The results also show the following usual statistics to assist in the evaluation of the methods (naturally, some of these statistics are not relevant to the explicit method):

Tol: accuracy requested for the integrator.
NTol: accuracy requested in the intermediate Newton scheme.
Newt failed: number of times the intermediate Newton scheme failed to converge, thus triggering a new stepsize.
Elocal failed: number of times the local error was rejected, which also triggers a new stepsize.

Table 1
Numerical results for Example 6.1 with $\omega = 1$, Error $= \max_n ||y_n - y(t_n)||_\infty$

Tol	NTol	Code	Time	Error	Time steps	Newt failed	Elocal failed	LUs	f evals	f_y evals	Linear solves
10^{-1}	10^{-4}	TIRK3	0.2900	3.3×10^{-12}	73	0	7	49	327	8	74
		RADAU5	0.1500	3.5×10^{-02}	146	0	35	132	821	36	177
	—	EFRK43	1.3620	1.4×10^{-03}	2495	—	548	—	11928	—	—
10^{-2}	10^{-5}	TIRK3	0.5010	0.9×10^{-11}	142	0	33	131	707	34	143
		RADAU5	0.1810	7.1×10^{-03}	177	0	29	117	942	30	215
	—	EFRK43	1.3320	1.6×10^{-04}	2442	—	530	—	11681	—	—
10^{-3}	10^{-6}	TIRK3	0.5910	3.7×10^{-12}	170	0	31	139	811	32	171
		RADAU5	0.2200	1.3×10^{-03}	232	0	31	165	1206	32	282
	—	EFRK43	1.3920	4.0×10^{-05}	2549	—	571	—	12175	—	—

Time steps: total number of all successful, Newt failed, and Elocal failed steps.
f evals: number of function evaluations.
f_y *evals*: number of times the Jacobian matrix was formed.
LUs: number of LU decompositions.
Linear solves: number of LU backsolves.

6.1. Linear Kramarz problem

It is represented by the second-order IVP (cf., e.g., [22,13])

$$\boldsymbol{y}''(t) = \begin{pmatrix} 2498 & 4998 \\ -2499 & -4999 \end{pmatrix} \boldsymbol{y}(t), \quad \boldsymbol{y}(0) = \begin{pmatrix} 2 \\ -1 \end{pmatrix}, \quad \boldsymbol{y}'(0) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad 0 \leqslant t \leqslant 100,$$

whose exact solution is $\boldsymbol{y}(t) = (2\cos(t), -\cos(t))^{\mathrm{T}}$. This system is stiff with $\lambda_1 = -1$, $\lambda_2 = -2500$ as its eigenvalues. Although EFRK43 is highly effective on non-stiff problems, the fact that it has a bounded stability region makes it unsuitable for solving stiff problems, even when the problem is periodic. Since TIRK3 is A-stable, we expect it to give better results than EFRK43 on this problem.

Numerical results are presented in Table 1. We see indeed that due to its small stability region, EFRK43 has to take small stepsizes and so uses a larger number of steps. In contrast, TIRK3 gives highly accurate results with fewer steps. In theory, TIRK3 should be exact to machine precision on this problem, but in practice, there is a downside in using the same Jacobian for different points $\{c_1 h, c_2 h, c_3 h\}$ and so the stepsize has to be kept small enough to achieve the desired accuracy.

6.2. Nonlinear Strehmel–Weiner problem

It is represented by the second-order IVP (cf., e.g., [6])

$$y_1''(t) = (y_1(t) - y_2(t))^3 + 6368 y_1(t) - 6384 y_2(t) + 42\cos(10t), \quad 0 \leqslant t \leqslant 10,$$

$$y_2''(t) = -(y_1(t) - y_2(t))^3 + 12768 y_1(t) - 12784 y_2(t) + 42\cos(10t),$$

with the exact solution $y_1(t) = y_2(t) = \cos(4t) - \cos(10t)/2$.

Numerical results are presented in Table 2. Here again, EFRK43 has to use small stepsizes, unlike TIRK3 and RADAU5 that can take larger stepsizes and still give more accurate results. For this problem, TIRK3 is at least as good as RADAU5 and much better than EFRK43 in terms of global error and number of function evaluations.

Table 2
Numerical results for Example 6.2 with $\omega = 4$, Error $= \max_n \|y_n - y(t_n)\|_\infty$

Tol	NTol	Code	Time	Error	Time steps	Newt failed	Elocal failed	LUs	f evals	f_y evals	Linear solves
10^{-2}	10^{-5}	TIRK3	0.5910	2.5×10^{-4}	166	0	32	124	907	33	203
		RADAU5	0.1900	2.2×10^{-4}	163	0	27	132	853	27	194
	—	EFRK43	0.2500	3.7×10^{-4}	431	—	99	—	2057	—	—
10^{-3}	10^{-6}	TIRK3	0.8310	6.6×10^{-6}	242	0	37	158	1288	38	298
		RADAU5	0.2210	4.4×10^{-4}	237	0	34	150	1208	35	277
	—	EFRK43	0.2210	3.0×10^{-4}	346	—	16	—	1715	—	—
10^{-4}	10^{-7}	TIRK3	1.0910	7.0×10^{-6}	319	0	36	200	1682	37	405
		RADAU5	0.3210	6.0×10^{-6}	326	0	37	214	1639	38	387
	—	EFRK43	0.3600	2.7×10^{-5}	620	—	22	—	3079	—	—

Table 3
Error $= \max_{i=1,2} |y_i(T) - y_i^{\text{comput}}(T)|$ for $\beta = -3$, $\omega = 1$ at $T = 10$

Tol	NTol	Code	Time	Error	Time steps	Newt failed	Elocal failed	LUs	f evals	f_y evals	Linear solves
10^{-1}	10^{-4}	TIRK3	0.0400	5.4×10^{-6}	10	0	1	10	47	2	11
		RADAU5	0.0200	9.4×10^{-4}	12	0	1	10	58	2	14
	—	EFRK43	0.0300	1.5×10^{-5}	11	—	0	—	56	—	—
10^{-2}	10^{-5}	TIRK3	0.1010	4.5×10^{-4}	23	0	5	13	113	6	26
		RADAU5	0.0200	1.3×10^{-4}	14	0	1	12	66	2	16
	—	EFRK43	0.0300	1.1×10^{-5}	12	—	0	—	61	—	—
10^{-3}	10^{-6}	TIRK3	0.0900	8.3×10^{-8}	19	0	2	14	88	3	21
		RADAU5	0.0500	2.4×10^{-3}	32	0	6	17	157	7	37
	—	EFRK43	0.0210	5.7×10^{-6}	20	—	2	—	99	—	—

6.3. A nearly sinusoidal problem

Consider the system (see [24, p. 354], [15])

$$y_1' = -2y_1 + y_2 + 2\sin(t),$$

$$y_2' = -(\beta + 2)y_1 + (\beta + 1)(y_2 + \sin(t) - \cos(t)).$$

This system has been used with $\beta = -3$ and $\beta = -1000$ in order to illustrate the phenomenon of stiffness. If the initial conditions are $y_1(0) = 2$ and $y_2(0) = 3$ the exact solution is β-independent and reads

$$y_1(t) = 2\exp(-t) + \sin(t),$$

$$y_2(t) = 2\exp(-t) + \cos(t).$$

When $\beta = -3$, due to the fact that the system is not stiff, EFRK43 performs quite well and is better than TIRK3 and RADAU5 for some cases. Overall, TIRK3 is at least as good as both RADAU5 and EFRK43. The numerical results for $\beta = -3$ are presented in Table 3.

The numerical results for $\beta = -1000$ are presented on Table 4. Looking at the table it is clear that when the system is stiff, TIRK3 becomes superior to EFRK43 by far. In fact, TIRK3 is better than both RADAU5 and EFRK43 on two key points, namely the global accuracy and the number of function evaluations.

All the computations were carried out in double-precision arithmetic on a PC computer with an Intel Centrino CPU of 1.7 GHz and 512 MB RAM.

Table 4
Error $= \max_{i=1,2}|y_i(T) - y_i^{\text{comput}}(T)|$ for $\beta = -1000$, $\omega = 1$ at $T = 10$

Tol	NTol	Code	Time	Error	Time steps	Newt failed	Elocal failed	LUs	f evals	f_y evals	Linear solves
10^{-1}	10^{-4}	TIRK3	0.0800	1.0×10^{-6}	13	0	2	12	61	3	14
		RADAU5	0.0300	3.3×10^{-5}	12	0	1	10	58	2	14
	—	EFRK43	1.7930	3.9×10^{-3}	3342	—	10	—	16701	—	—
10^{-2}	10^{-5}	TIRK3	0.0600	1.6×10^{-7}	16	0	2	15	76	3	18
		RADAU5	0.0800	1.1×10^{-5}	22	0	5	22	112	6	26
	—	EFRK43	1.8220	5.2×10^{-4}	3454	—	10	—	17261	—	—
10^{-3}	10^{-6}	TIRK3	0.0800	7.0×10^{-8}	21	0	3	18	98	4	23
		RADAU5	0.0500	1.3×10^{-6}	28	0	6	27	141	7	33
	—	EFRK43	1.8830	2.5×10^{-5}	3512	—	8	—	17553	—	—

7. Conclusion

We have studied the family of TIRK methods and established under which conditions they are A-stable. Experiments showed that they can achieve very high accuracy, higher than RADAU5.

While the A-stability property suggests that TIRK methods can integrate the exact solution of certain periodic ODE problems using any stepsize, there are however a few limitations in practice due to the Newton scheme. This dependency puts a restriction on the stepsize. Indeed, the implicit nature of the methods means that we have to use Newton iterations to solve non-linear systems to retrieve the intermediate stage values. The stepzise can therefore not exceed one period because these Newton iterations use the same approximated Jacobian matrix over the interval of one step for the points $\{c_i h\}_{i=1}^{s}$—which presupposes that the derivative of the exact solution at these points should not vary significantly.

In addition, the overall accuracy hinges on the accuracy tolerance in these Newton iterations. This bounds the final accuracy of the numerical results, causing it not to always be as high as we might expect. However, owing to their good stability properties, we saw in the experiments that these implicit trigonometric methods were still efficient on nearly sinusoidal problems or sinusoidal problems with an approximated frequency.

There is nevertheless one particular shortcoming of this class of methods in that only one frequency is considered over time, whereas the frequency can vary or different components of the solution can have their own frequency. Although it comes to mind that if the problem contains many frequencies, one can use a representative frequency such as a rough common divisor of these frequencies, the representative frequency, if any, may be very small and in this case the coefficients of the method converge to a classical method as we showed. As for problems for which the frequency varies over time, these require techniques to find the frequency adaptively during computation.

In summary, the theory developed in this study as well as the implementation have shown that the new class of TIRK methods have some interesting properties that may be helpful in designing and improving numerical methods for oscillatory ODE problems. The study has concluded by pointing out other aspects needing further study.

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