SIAM J. NUMER. ANAL.
Vol. 26, No. 1, pp. 214-229, February 1989

012

PHASE-LAG ANALYSIS OF IMPLICIT RUNGE-KUTTA METHODS*

P. J. VAN DER HOUWEN† AND B. P. SOMMEIJER†

Abstract. We analyse the phase errors introduced by implicit Runge-Kutta methods when a linear inhomogeneous test equation is integrated. It is shown that the homogeneous phase errors dominate if long interval integrations are performed. Homogeneous dispersion relations for the special class of DIRK methods are derived and a few high-order dispersive DIRK methods are constructed. These methods are applied to systems of linear differential equations with oscillating solutions and compared with the "conventional" DIRK methods of Nørsett and Crouzeix.

Key words. numerical analysis, ordinary differential equations, Runge-Kutta methods, periodic solutions

AMS(MOS) subject classification. 65L05

1. Introduction. In this paper, special diagonally implicit Runge-Kutta (DIRK) methods will be constructed for integrating systems of ODEs of the form

$$\frac{dy(t)}{dt}=f(t, y(t)), \qquad y(t_0)=y_0, \tag{1.1}$$

when we know in advance that the solution is oscillating. Analogously to a generally adopted approach in the phase-lag analysis of numerical methods for second-order equations with oscillating solutions, we use the equation (cf. [1], [3], [4], [7], [8], [12]-[16])

$$\frac{dy(t)}{dt}=i\omega y(t)+\delta\, e^{i\omega_p t}, \quad \delta, \omega, \omega_p \in \mathbb{R}, \quad \omega \neq \omega_p \tag{1.2}$$

as a test equation. Here ω represents a natural (or eigen) frequency of the system and ω_p represents the frequency of the forced solution component.

In § 2, we start by deriving explicit expressions for the phase lag introduced by general, implicit Runge-Kutta (RK) methods. The phase lag is composed of two parts: the *homogeneous* phase lag corresponding to the eigenmodes in the solution, and the *inhomogeneous* phase lag corresponding to the forced solution component. We will show that in calculations over long intervals of integration, the homogeneous phase lag tends to increase linearly, whereas the inhomogeneous phase error is constant. For this reason, we concentrate on the reduction of *homogeneous phase errors.*

In § 3, we introduce the concept of a *qth order dispersive stability function,* and we show that such a stability function generates Runge-Kutta methods that have homogeneous phase errors of order q.

From § 4 on, we confine our considerations to DIRK methods. We first derive the (dispersion) relations specifying a qth order dispersive stability function (we remark that for *explicit* Runge-Kutta methods these relations can be found in [8]). It is shown that there exists a one-parameter family of m-stage, pth order consistent DIRK methods with homogeneous phase errors of order $q=2(m-\lfloor p/2\rfloor)$. In § 5, the dispersion relations are solved for one-, two-, three-, and four-stage DIRK methods and the resulting stability functions are constructed. These functions are dispersive of order $q=2m$. The two-stage stability function turns out to be identical with the stability function of the well-known DIRK method of Nørsett [10].

* Received by the editors May 27, 1986; accepted for publication (in revised form) January 19, 1988.
† Centre for Mathematics and Computer Science, P.O. Box 4079, 1009 AB Amsterdam, the Netherlands.

The actual construction of highly dispersive DIRK methods is given in § 6. Here, a three- and a four-stage method are presented that are both A-stable and third-order consistent, and that have homogeneous dispersion order $q=6$ and $q=8$, respectively.

In § 7, these methods are applied to systems of linear differential equations in which the oscillating solution component is dominating. The results are in perfect agreement with the theory. Comparison with the DIRK methods of Nørsett [10] and Crouzeix [5] shows that the higher-order dispersive methods proposed in this paper produce much more accurate results than conventional DIRK methods.

Finally, we remark that stepsize control can be based on reference formulas of an explicit type that can be constructed along the lines indicated in [8].

2. The RK solution of the basic test equation. The general m-stage RK method for the system of ODEs (1.1) is given by

$$Y_{nj}=y_n+h\sum_{l=1}^{m} a_{jl}f(t_n+c_lh,\ Y_{nl}),\quad j=1,\cdots,m, \tag{2.1a}$$

$$y_{n+1}=y_n+h\sum_{j=1}^{m} b_jf(t_n+c_jh,\ Y_{nj}), \tag{2.1b}$$

where the RK parameters a_{jl}, b_j, and c_j are assumed to be real.

Application of the RK method (2.1) to the basic test equation (1.2) leads to the recursions

$$\begin{aligned} Y_{nj}&=y_n+iv\sum_{l=1}^{m} a_{jl}Y_{nl}+\delta h\, e^{i\omega_p t_n}\sum_{l=1}^{m} a_{jl}\,e^{ic_lv_p},\\ y_{n+1}&=y_n+iv\sum_{j=1}^{m} b_jY_{nj}+\delta h\, e^{i\omega_p t_n}\sum_{j=1}^{m} b_j\,e^{ic_jv_p}, \end{aligned} \tag{2.1'}$$

where we have set

$$v:=\omega h,\qquad v_p:=\omega_p h.$$

Introducing the matrix $A=(a_{jl})$ and the vectors $\mathbf{b}=(b_j)$, $\mathbf{c}=(c_j)$, $\mathbf{Y}_n=(Y_{nj})$, $\mathbf{e}_p=(\exp(ic_jv_p))$ and $\mathbf{e}=(1,\cdots,1)^T$, we can write (2.1') in the compact form

$$\mathbf{Y}_n=y_n\mathbf{e}+ivA\mathbf{Y}_n+\delta h\, e^{i\omega_p t_n}A\mathbf{e}_p,\qquad y_{n+1}=y_n+iv\mathbf{b}^T\mathbf{Y}_n+\delta h\, e^{i\omega_p t_n}\mathbf{b}^T\mathbf{e}_p. \tag{2.1''}$$

From (2.1'') a recursion for y_n can be derived:

$$y_{n+1}=[1+iv\mathbf{b}^T(I-ivA)^{-1}\mathbf{e}]y_n+\delta h\, e^{i\omega_p t_n}\mathbf{b}^T[I+iv(I-ivA)^{-1}A]\mathbf{e}_p. \tag{2.2}$$

It is convenient to define the rational functions (in z)

$$R(z):=1+z\mathbf{b}^T(I-zA)^{-1}\mathbf{e},\qquad Q(z,\ iv_p):=\mathbf{b}^T(I-zA)^{-1}\mathbf{e}_p, \tag{2.3}$$

so that the Runge–Kutta recursion for the test equation (1.2) is given by

$$y_{n+1}=R(iv)y_n+\delta hQ(iv,\ iv_p)\,e^{i\omega_p t_n}. \tag{2.2'}$$

$R(z)$ is known as the *stability function* of the RK method.

Let us write the solution of (2.2') in the explicit form

$$y_n=\tilde a_1^n[y_0-\tilde a_0\,e^{i\omega_p t_0}]+\tilde a_0\,e^{i\omega_p t_n}. \tag{2.4a}$$

Then, by substitution into (2.2'), we derive

$$\tilde a_1=R(iv),\qquad \tilde a_0=\frac{\delta hQ(iv,\ iv_p)}{e^{iv_p}-R(iv)}. \tag{2.4b}$$

For the exact solution of the basic test equation we have

$$y(t_n) = a_1^n[y(t_0) - a_0 e^{i\omega_p t_0}] + a_0 e^{i\omega_p t_n}, \tag{2.5a}$$

$$a_1 := \exp(iv), \qquad a_0 := \frac{\delta h}{iv_p - iv}. \tag{2.5b}$$

We shall compare the phases of the quantities a_j and $\tilde{a}_j$ with the aim to derive conditions for high-order phase errors.

DEFINITION 2.1. In the RK scheme (2.1) the functions

$$\phi_1(v) := \arg\left[\frac{a_1}{\tilde{a}_1}\right] = v - \arg[R(iv)],$$

$$\phi_0(v, v_p) := \arg\left[\frac{a_0}{\tilde{a}_0}\right] = \arg\left[\frac{\exp(iv_p) - R(iv)}{(iv_p - iv)Q(iv, iv_p)}\right]$$

respectively, are called the *homogeneous* and *inhomogeneous dispersion* (or *phase error, phase lag*). If $\phi_1 = O(h^{q+1})$ as $h \to 0$, with ω constant, then the method is said to have *homogeneous dispersion order q*. If $\phi_0 = O(h^q)$ as $h \to 0$, with ω and ω_p constant, then the method is said to have *inhomogeneous dispersion order q*.

Remark. We mention that the definition of *homogeneous dispersion* given above is identical to the one used in [8]. Furthermore, it is closely related to the definition of phase lag as given by Brusa and Nigro [1]. Their formulation is in terms of accurately approximating the exponentials in the exact solution by the eigenvalues of the amplification matrix of the numerical scheme. To be more precise, writing the roots of the characteristic equation in the form

$$\exp(\{-a(v) \pm ib(v)\}v),$$

they define the *phase lag* (or *frequency distortion*) as the modulus of the leading term in the expansion of $b-1$ in powers of v.

Furthermore, our definition of *inhomogeneous dispersion* is completely analogous to the one used in the literature (see e.g. [7], [13]-[15]).

In comparing the numerical solution (2.4a) and the exact solution (2.5a), we observe that the (complex) numbers $\tilde{a}_1$ and a_1 are raised to the power n. This means that we may expect a linear accumulation of the phase error due to homogeneous dispersion, since $\arg(a_1^n) - \arg(\tilde{a}_1^n) = n(\arg(a_1) - \arg(\tilde{a}_1)) = n\phi_1$. On the other hand, the phase error introduced by the inhomogeneous term (i.e., the difference in the arguments of a_0 and $\tilde{a}_0$) is independent of n and, consequently, constant in time.

Therefore, in computations with fixed stepsize h and large integration intervals the homogenous dispersion is the most crucial source of phase errors; it causes the numerical solution to become increasingly out of phase with the exact solution. Since we usually want a solution that has an error that does not change too much over the interval of integration, we will concentrate on the reduction of the magnitude of $\phi_1(\nu)$. Consequently, when a method is called dispersive of order q we always mean that the method has *homogeneous* dispersion order q.

2.1. Derivation of the order of dispersion. In the derivation of the functions ϕ_j we need the functions R and Q defined in (2.3). In order to evaluate R and Q the following lemma may be helpful.

LEMMA 2.1. *Let M be a nonsingular $m \times m$ matrix, and $\mathbf{v}$ and $\mathbf{w}$ m-dimensional vectors. Then*

$$\mathbf{v}^T M^{-1} \mathbf{w} = \frac{\det[M + \mathbf{w}\mathbf{v}^T]}{\det[M]} - 1.$$

Proof. Let $\mathbf{x} := M^{-1}\mathbf{w}$ and $x_{m+1} := 1 + \mathbf{v}^T\mathbf{x}$; then $(\mathbf{x}^T, x_{m+1})$ satisfies the system of $m+1$ equations:

$$\begin{bmatrix} M_{11} & \cdots & M_{1m} & 0 \\ \vdots & & \vdots & \vdots \\ M_{m1} & \cdots & M_{mm} & 0 \\ -v_1 & \cdots & -v_m & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_m \\ x_{m+1} \end{bmatrix} = \begin{bmatrix} w_1 \\ \vdots \\ w_m \\ 1 \end{bmatrix},$$

where M_{jl} are the entries of M, and x_j, v_j, w_j the components of $\mathbf{x}$, $\mathbf{v}$, $\mathbf{w}$. By Cramer's rule we may write

$$x_{m+1} := 1 + \mathbf{v}^T M^{-1}\mathbf{w} = \frac{\det[N]}{\det[M]},$$

with

$$N = \begin{bmatrix} M & \mathbf{w} \\ -\mathbf{v}^T & 1 \end{bmatrix}.$$

Subtracting the row vector $w_i(-\mathbf{v}^T, 1)$ from the ith row of $N (i = 1, \cdots, m)$ leads to

$$\det[N] = \det[M + \mathbf{w}\mathbf{v}^T]$$

which proves the lemma. □

Using this lemma we derive from (2.3) for $R(z)$ the familiar expression (cf. [11, p. 132])

$$R(z) = \frac{\det[I - zA + \mathbf{e}\cdot\mathbf{b}^T z]}{\det[I - zA]}, \tag{2.6a}$$

and for $Q(z)$ we obtain

$$Q(z, iv_p) = \frac{\det[I - zA + \mathbf{e}_p\cdot\mathbf{b}^T]}{\det[I - zA]} - 1. \tag{2.6b}$$

Remark. We mention that the homogeneous and inhomogeneous dispersion orders may be (quite) different. To illustrate this, consider the backward Euler method [9] for which it can straightforwardly be verified that

$$\phi_1(v) = v - \arctan(v), \qquad \phi_0(v, v_p) = \arctan\left(\frac{1 - \cos(v_p)}{v - \sin(v_p)}\right),$$

showing that the backward Euler method has homogeneous and inhomogeneous orders of dispersion $q = 2$ and $q = 1$, respectively.

For the trapezoidal rule [9] the situation is different. Here we obtain

$$\phi_1(v) = v - \arctan\left[\frac{v}{1 - \frac{1}{4}v^2}\right], \qquad \phi_0(v, v_p) = \arg\left[\frac{2\tan(v_p/2) - v}{v_p - v}\right] = 0.$$

Hence, the order of the homogeneous dispersion is $q = 2$, whereas the inhomogeneous dispersion is of infinite order, which is due to the symmetry of the trapezoidal rule (see Thomas [15]).

3. Dispersive stability functions. Ideally, the stability function $R(z)$ of an RK method should be such that $\phi_1(v) := v - \arg(R(iv))$ vanishes identically. Although this will not be possible, it is interesting to characterize the class of functions for which $\phi_1(v)$ does vanish identically.

DEFINITION 3.1. A function $\tilde{R}(z)$ is said to be in class $\mathscr{D}_\infty$ if $\phi_1(v) := v - \arg(\tilde{R}(iv)) \equiv 0$ on $\mathbb{R}$, or equivalently,

$$\operatorname{Im}(\tilde{R}(iv)) \equiv \tan(v)\operatorname{Re}(\tilde{R}(iv)) \quad \text{on } \mathbb{R}. \tag{3.1}$$

THEOREM 3.1. *A rational function $\tilde{R}(z)$ with real coefficients is in class $\mathscr{D}_\infty$ if and only if its Taylor expansion is of the form*

$$\tilde{R}(z) = \sum_{j=0}^{\infty} \left[\tilde{\beta}_{2j} + z \sum_{l=0}^{j} (-1)^{l+j} \gamma_{2(j-l)} \tilde{\beta}_{2l} \right] z^{2j}, \tag{3.2}$$

where $\tilde{\beta}_0 = 1$ and $\tilde{\beta}_2, \tilde{\beta}_4, \cdots$ are arbitrary parameters in $\mathbb{R}$, and where the γ_{2l} are the coefficients in the Taylor expansion

$$\tan(z) = z \sum_{l=0}^{\infty} \gamma_{2l} z^{2l}. \tag{3.3}$$

Proof. It is straightforwardly verified that $\arg(\tilde{R}(iv)) \equiv v$ for $v \in \mathbb{R}$ and all real $\tilde{\beta}_{2j}$, $j > 0$. Conversely, substituting a formal Taylor expansion for $\tilde{R}$ into (3.1) leads to expressions for the Taylor coefficients that are readily identified with those of (3.2). □

As an illustration, we give the first few terms of the expansion (3.2) explicitly:

$$\begin{aligned} \tilde{R}(z) = 1 + z + \tilde{\beta}_2 z^2 + \left(\tilde{\beta}_2 - \frac{1}{3}\right) z^3 + \tilde{\beta}_4 z^4 + \left(\tilde{\beta}_4 - \frac{1}{3}\tilde{\beta}_2 + \frac{2}{15}\right) z^5 \\ + \tilde{\beta}_6 z^6 + \left(\tilde{\beta}_6 - \frac{1}{3}\tilde{\beta}_4 + \frac{2}{15}\tilde{\beta}_2 - \frac{17}{315}\right) z^7 \\ + \tilde{\beta}_8 z^8 + \left(\tilde{\beta}_8 - \frac{1}{3}\tilde{\beta}_6 + \frac{2}{15}\tilde{\beta}_4 - \frac{17}{315}\tilde{\beta}_2 + \frac{62}{2835}\right) z^9 + \cdots. \end{aligned} \tag{3.2'}$$

A trivial example of a function from $\mathscr{D}_\infty$ is given by $\exp(z)$; it can be written in the form (3.2) by defining $\tilde{\beta}_{2j} := 1/(2j)!$.

It is convenient to introduce the notion of *consistent* and *dispersive* stability functions.

DEFINITION 3.2. (a) A given stability function $R(z)$ is called *consistent of order* p if

$$R(z) = \exp(z) + O(z^{p+1}).$$

(b) It is called *dispersive of order* q (or *belonging to class* $\mathscr{D}_q$) if there exists a function $\tilde{R} \in \mathscr{D}_\infty$ such that

$$R(z) = \tilde{R}(z) + O(z^{q+1}).$$

This definition is justified by the following theorem.

THEOREM 3.2. (a) *A pth-order consistent* RK *method possesses a pth-order consistent stability function.*

(b) *An* RK *method has homogeneous dispersion order q if and only if its stability function is dispersive of order q (belongs to $\mathscr{D}_q$).*

Proof. Assertion (a) of the theorem is well known (see, e.g., [6]).

The *sufficient* part of assertion (b) is proved as follows. Let $R \in \mathscr{D}_q$, i.e., $R(z) = \tilde{R}(z) + O(z^{q+1})$ with $\tilde{R} \in \mathscr{D}_\infty$, then

$$\begin{aligned} \phi_1(v) := v - \arg(R(iv)) &= [v - \arg(R(iv))] - [v - \arg(\tilde{R}(iv))] \\ &= \arg(\tilde{R}(iv)/R(iv)) = \arg(1 + O(v^{q+1})) = O(v^{q+1}), \end{aligned}$$

showing that the RK method has homogeneous dispersion order q.

Conversely, let $\phi_1(v) = O(v^{q+1})$; then

$$\operatorname{Im}(R(iv)) = \tan(v) \operatorname{Re}(R(iv)) + O(v^{q+1}).$$

On substitution of the Taylor expansion of the given function $R(z)$ into this last equation and using (3.3), we can show that the Taylor coefficients of $R(z)$ can be identified with those of (3.2) up to order q. Hence, there exists a function $\tilde{R} \in \mathcal{D}_\infty$ such that $R - \tilde{R} = O(z^{q+1})$. □

Evidently, any pth-order consistent RK method has homogeneous dispersion order $q \geqq p$. However, if p is *odd*, then we automatically get a one order higher homogeneous phase error.

THEOREM 3.3. *An* RK *method of consistency order* $p = 2p_0 + 1$ *has homogeneous dispersion order* $q \geqq 2p_0 + 2$.

Proof. According to Theorem 3.2(a) and Definition 3.2(a), the stability function $R(z)$ has a Taylor expansion of the form

$$R(z) = 1 + z + \frac{1}{2} z^2 + \cdots + \frac{1}{(2p_0+1)!} z^{2p_0+1} + \beta_{2p_0+2} z^{2p_0+2} + \beta_{2p_0+3} z^{2p_0+3} + \cdots, \tag{3.4}$$

where the coefficients β_j, $j > 2p_0 + 1$ are expressions in terms of the RK parameters.

Next we consider the function $\tilde{R}(z)$ with $\tilde{\beta}_{2l} = 1/(2l)!$ for $l \leqq p_0$, to obtain

$$\tilde{R}(z) = \sum_{j=0}^{p_0} \left[\frac{1}{(2j)!} + z \sum_{l=0}^{j} (-1)^{l+j} \gamma_{2(j-l)} \frac{1}{(2l)!} \right] z^{2j} + \tilde{\beta}_{2p_0+2} z^{2p_0+2} + O(z^{2p_0+3}). \tag{3.5}$$

Furthermore, using that $e^z = \sum_{j=0}^{\infty} z^j/j!$ can be written in the form (3.2) and equating the coefficients of z^{2j+1} in both expansions, we obtain the relation

$$\sum_{l=0}^{j} (-1)^{l+j} \gamma_{2(j-l)} \frac{1}{(2l)!} = \frac{1}{(2j+1)!}. \tag{3.6}$$

Finally, by setting $\tilde{\beta}_{2p_0+2} = \beta_{2p_0+2}$ we may conclude from (3.4)-(3.6) that $R(z) - \tilde{R}(z) = O(z^{2p_0+3})$, which proves the theorem. □

4. Derivation of dispersion relations. In [8] dispersion relations have been derived for polynomial stability functions. In this paper we consider stability functions of the form

$$R(z) = \frac{\sum_{j=0}^{m} \alpha_j z^j}{(1+\alpha z)^m}, \qquad \alpha, \alpha_0, \cdots, \alpha_m \in \mathbb{R}. \tag{4.1}$$

If $\alpha = 0$ this function reduces to a polynomial and the results obtained in [8] apply. For instance, the maximal attainable order of dispersion for polynomial stability functions is given by

$$\bar{q} := 2\left(m - p + \left\lfloor \frac{p+1}{2} \right\rfloor\right) = 2\left(m - \left\lfloor \frac{p}{2} \right\rfloor\right). \tag{4.2}$$

In this section, it will be shown that in some cases this order of dispersion can be raised to $q = \bar{q} + 2$ by a judicious choice of α. To that end we need the dispersion relations for stability functions of the nonpolynomial form (4.1). In principle, these relations can be obtained from the relations derived for polynomial stability functions. By expanding (4.1) in a Taylor series of the form

$$R(z) = \sum_{j=0}^{\infty} \beta_j z^j,$$

we find that the β_j are polynomials in α with coefficients that are linear in the α_j, for example,

$$\beta_0 = \alpha_0, \quad \beta_1 = \alpha_1 - \alpha_0 \binom{m}{1} \alpha, \quad \beta_2 = \alpha_2 - \alpha_1 \binom{m}{1} \alpha + \alpha_0 \left[\binom{m}{1}^2 - \binom{m}{2} \right] \alpha^2.$$

We now use the dispersion relations derived in [8] for stability functions of the form

$$R(z)=\sum_{j=0}^{m}\beta_j z^j.$$

These dispersion relations are linear relations in terms of the β_j, so that by substituting our β_j-expressions, we obtain dispersion relations for stability functions of the form (4.1) that are linear in α_j but polynomial in α.

The approach outlined above leads to complicated formulas. Therefore, we prefer to follow an alternative approach that expresses the dispersion relations in terms of α and the parameters $\tilde{\beta}_j$ introduced in Theorem 3.1.

First of all we remark that q may be assumed to be even. This follows from the results obtained in § 3 (see especially Theorem 3.3).

In the following it is convenient to introduce the vectors

$$\text{(4.3a)}\qquad \begin{aligned}\tilde{\boldsymbol{\beta}}_q &:= (\tilde{\beta}_0,\tilde{\beta}_2,\tilde{\beta}_4,\cdots,\tilde{\beta}_q)^T\\ &=\left(1,\frac{1}{2!},\frac{1}{4!},\cdots,\frac{1}{\tilde{p}!},\tilde{\beta}_{\tilde{p}+2},\cdots,\tilde{\beta}_q\right)^T, \qquad \tilde{p}:=2\left[\frac{p}{2}\right],\end{aligned}$$

$$\text{(4.3b)}\qquad \boldsymbol{\alpha}_m := (\alpha_0,\alpha_1,\cdots,\alpha_m)^T,$$

the $(m+1)$ by $(q+1)$ matrix

$$\text{(4.3c)}\qquad B_1(\alpha):=\begin{bmatrix}\binom{m}{0}\alpha^0 & 0 & \cdots & 0 & 0 & \cdots & 0\\ \vdots & & & \vdots & & & \vdots\\ \binom{m}{m}\alpha^m & \binom{m}{m-1}\alpha^{m-1} & \cdots & \binom{m}{0}\alpha^0 & 0 & \cdots & 0\end{bmatrix},$$

the $(q-m)$ by $(q+1)$ matrix

(4.3d)

$$B_2(\alpha):=\begin{bmatrix}0 & \binom{m}{m}\alpha^m & \binom{m}{m-1}\alpha^{m-1} & \cdots & \binom{m}{1}\alpha & 1 & 0 & \cdots & 0\\ 0 & 0 & \binom{m}{m}\alpha^m & \binom{m}{m-1}\alpha^{m-1} & \cdots & \binom{m}{1}\alpha & 1 & \ddots & \vdots\\ \vdots & \ddots & \ddots & \ddots & & \ddots & \ddots & & 0\\ 0 & \cdots & 0 & \binom{m}{m}\alpha^m & \binom{m}{m-1}\alpha^{m-1} & \cdots & & \binom{m}{1}\alpha & 1\end{bmatrix}$$

and the $(q+1)$ by $(q/2+1)$ matrix

$$\text{(4.3e)}\qquad C:=\begin{bmatrix}1 & & & & & & \\ \gamma_0 & & & & & & \\ 0 & 1 & & & & & \\ -\gamma_2 & \gamma_0 & & & & & \\ 0 & 0 & 1 & & & & \\ \gamma_4 & -\gamma_2 & \gamma_0 & & & & \\ \vdots & & & & & & \\ 0 & & \cdots & 0 & 0 & 1 & \\ (-1)^{(q-2)/2}\gamma_{q-2} & & \cdots & \gamma_4 & -\gamma_2 & \gamma_0 & \\ 0 & & \cdots & 0 & 0 & 0 & 1\end{bmatrix}.$$

Here, p is the order of consistency of (4.1) and q is even. Moreover, to let the definition of the matrix $B_2(\alpha)$ be meaningful, we require its dimensions to be positive, i.e., $q>m$.

THEOREM 4.1. *Let p be the order of consistency of* (4.1) *and let q be an even integer* $>m$. *Then the stability function* (4.1) *is dispersive of order q if there exists a real vector* $\tilde{\boldsymbol{\beta}}_q$ *and a real* α *such that*

$$B_2(\alpha)C\tilde{\boldsymbol{\beta}}_q = \mathbf{0}, \tag{4.4a}$$

and if

$$\boldsymbol{\alpha}_m = B_1(\alpha)C\tilde{\boldsymbol{\beta}}_q. \tag{4.4b}$$

Proof. The Taylor expansion of the stability function is of the form

$$R(z) = \sum_{j=0}^{\infty} \beta_j z^j, \quad \beta_j := \frac{1}{j!} \quad \text{for } j = 0, 1, \cdots, p,$$

where the coefficients β_j, $j \geqq p+1$ are in $\mathbb{R}$. From (4.1) it follows that

$$\alpha_j - \sum_{l=0}^{j} \beta_l \binom{m}{j-l} \alpha^{j-l} = 0, \qquad j = 0, 1, \cdots, \tag{4.5}$$

where $\alpha_j := 0$ for $j > m$. Using the notation (4.3) and introducing the vector

$$\begin{aligned} \boldsymbol{\beta}_q &:= (\beta_0, \beta_1, \beta_2, \cdots, \beta_q)^T \\ &= \left(1, 1, \frac{1}{2!}, \cdots, \frac{1}{p!}, \beta_{p+1}, \cdots, \beta_q\right)^T, \end{aligned}$$

we deduce from Theorem 3.1 and (3.6) that $R \in \mathcal{D}_q$ if

$$\boldsymbol{\beta}_q = C\tilde{\boldsymbol{\beta}}_q. \tag{4.6}$$

It follows from (4.5) that (again using the notation (4.3))

$$\boldsymbol{\alpha}_m = B_1(\alpha)\boldsymbol{\beta}_q, \qquad B_2(\alpha)\boldsymbol{\beta}_q = \mathbf{0}.$$

On substitution of (4.6) we arrive at the relations (4.4). □

COROLLARY 4.1. *Let* (4.1) *be consistent of order p and let* $q = \bar{q} = 2(m - \lfloor p/2 \rfloor)$ (*cf.* (4.2)). *Then* (4.4) *determines a one-parameter family* $R(z; \alpha)$ *of stability functions in* $\mathcal{D}_{\bar{q}}$.

Proof. For each α, (4.4a) represents a linear system of $q-m$ equations for the $(q-\tilde{p})/2$ unknowns $\tilde{\beta}_{\tilde{p}+2}, \tilde{\beta}_{\tilde{p}+4}, \cdots, \tilde{\beta}_q$ with $\tilde{p} := 2\lfloor p/2 \rfloor$. By choosing $q = 2m - \tilde{p} = \bar{q}$ the number of unknowns equals the number of equations. The parameter α can be chosen such that the matrix of coefficients in this system is nonsingular, and hence a unique solution exists. Then, on substitution of $q = \bar{q}$ and $\tilde{\boldsymbol{\beta}}_q = \tilde{\boldsymbol{\beta}}_{\bar{q}}$ into (4.4b), the vector $\boldsymbol{\alpha}_m$ can be calculated in terms of the parameter α. According to Theorem 4.1, the resulting stability function is dispersive of order $\bar{q}$, i.e., it lies in $\mathcal{D}_{\bar{q}}$. □

It has already been observed that the dispersion order can sometimes be raised by two by a judicious choice of α. This happens when there exists a real value α such that (4.4a) can be satisfied for $q = \bar{q}+2$. To obtain a nontrivial solution for this homogeneous system we must require a vanishing determinant. This results in a polynomial equation in α, and it is not guaranteed that a solution α in $\mathbb{R}$ exists.

5. Construction of highly dispersive stability functions.

5.1. The case $m = 1$, $p = 1$. Let us try to achieve order of dispersion $q = 4$. The dispersion relations (4.4a) reduce to

$$\begin{bmatrix} \gamma_0\alpha & 1 & 0 \\ -\gamma_2 & \alpha+\gamma_0 & 0 \\ -\gamma_2\alpha & \gamma_0\alpha & 1 \end{bmatrix} \begin{bmatrix} 1 \\ \tilde{\beta}_2 \\ \tilde{\beta}_4 \end{bmatrix} = \mathbf{0}. \tag{5.1}$$

The first relation is satisfied if $\tilde{\beta}_2 = -\gamma_0\alpha$; the second relation reads

$$\gamma_0\alpha^2 + \gamma_0^2\alpha + \gamma_2 = 0,$$

which has no real solution (recall that $\gamma_0 = 1$, $\gamma_2 = \frac{1}{3}$). Hence, $q = 2$ and, according to (4.4b), $\alpha_1 = 1 + \alpha$. Thus, we have the first-order consistent and second-order dispersive family

$$R(z;\, \alpha) = \frac{1+(1+\alpha)z}{(1+\alpha z)}. \tag{5.2}$$

5.2. The case $m = 2$, $p = 1$. We try $q = 6$; (4.4a) reads

$$\begin{bmatrix} \gamma_0\alpha^2-\gamma_2 & 2\alpha+\gamma_0 & 0 & 0 \\ -2\gamma_2\alpha & \alpha^2+2\gamma_0\alpha & 1 & 0 \\ -\gamma_2\alpha^2+\gamma_4 & \gamma_0\alpha^2-\gamma_2 & 2\alpha+\gamma_0 & 0 \\ 2\gamma_4\alpha & -2\gamma_2\alpha & \alpha^2+2\gamma_0\alpha & 1 \end{bmatrix} \begin{bmatrix} 1 \\ \tilde{\beta}_2 \\ \tilde{\beta}_4 \\ \tilde{\beta}_6 \end{bmatrix} = \mathbf{0}. \tag{5.3}$$

The first two equations are solved by

$$\tilde{\beta}_2 = \frac{\gamma_2-\gamma_0\alpha^2}{\gamma_0+2\alpha}, \qquad \tilde{\beta}_4 = 2\gamma_2\alpha - \alpha\frac{(2\gamma_0+\alpha)(\gamma_2-\gamma_0\alpha^2)}{\gamma_0+2\alpha}. \tag{5.4a}$$

The third equation then becomes, upon substitution of $\gamma_0 = 1$, $\gamma_2 = \frac{1}{3}$, $\gamma_4 = 2/15$,

$$90\alpha^5 + 180\alpha^4 + 150\alpha^3 + 60\alpha^2 + 12\alpha + 1 = 0,$$

possessing the *real* root

$$\alpha = -.28416\,43597\cdots. \tag{5.4b}$$

The fourth equation expresses $\tilde{\beta}_6$ in terms of $\tilde{\beta}_2$, $\tilde{\beta}_4$, and α. The parameter vector $\boldsymbol{\alpha}_2$ can now be computed by means of (4.4b). The resulting stability function reads

$$R(z;\, \alpha) = \frac{1+(2\alpha+1)z+(\alpha^3+2\alpha^2+\alpha+\frac{1}{6})z^2/(\alpha+\frac{1}{2})}{(1+\alpha z)^2}. \tag{5.5}$$

It is sixth-order dispersive if α is given by (5.4b) and fourth-order dispersive otherwise.

5.3. The case $m = 2$, $p = 3$. The corresponding dispersion relations can be derived from (5.3) by setting $\tilde{\beta}_2 = \frac{1}{2}$. From (5.4a) it then follows that α should satisfy

$$\alpha^2 + \alpha + \tfrac{1}{6} = 0,$$

i.e., $\alpha = -\frac{1}{2} \pm \sqrt{3}/6$. The resulting third-order consistent, fourth-order dispersive stability function given by

$$R(z;\, \alpha) = \frac{1+(2\alpha+1)z+(\alpha^2+2\alpha+\frac{1}{2})z^2}{(1+\alpha z)^2}, \qquad \alpha = -\frac{1}{2} \pm \frac{1}{6}\sqrt{3}, \tag{5.6}$$

is identical with the stability function considered by Nørsett [10].

5.4. The case $m = 3$, $p = 3$. The dispersion relations (4.4a) with $q = 6$ assume the form

$$\begin{bmatrix} \gamma_0\alpha^3 - 3\gamma_2\alpha & 3\alpha(\alpha+\gamma_0) & 1 & 0 \\ -3\gamma_2\alpha^2 + \gamma_4 & \alpha^3 + 3\gamma_0\alpha^2 - \gamma_2 & 3\alpha + \gamma_0 & 0 \\ \alpha(-\gamma_2\alpha^2 + 3\gamma_4) & \alpha(\gamma_0\alpha^2 - 3\gamma_2) & 3\alpha(\alpha+\gamma_0) & 1 \end{bmatrix} \begin{bmatrix} 1 \\ \frac{1}{2} \\ \tilde{\beta}_4 \\ \tilde{\beta}_6 \end{bmatrix} = \mathbf{0}.$$

The first equation is solved by

$$\tilde{\beta}_4 = -\gamma_0\alpha^3 + 3\gamma_2\alpha - \tfrac{3}{2}\alpha(\alpha + \gamma_0), \tag{5.7a}$$

and the second equation becomes

$$90\alpha^4 + 150\alpha^3 + 75\alpha^2 + 15\alpha + 1 = 0.$$

This equation has the real solutions

$$\alpha^{(1)} = -.13633\,37707\cdots, \qquad \alpha^{(2)} = -.97567\,45887\cdots. \tag{5.7b}$$

The last equation expresses $\tilde{\beta}_6$ in terms of α and $\tilde{\beta}_4$ so that, by (4.4b), the parameter vector $\boldsymbol{\alpha}_3$ can be computed. The resulting stability function is given by

$$R(z;\alpha) = \frac{1 + (3\alpha+1)z + (3\alpha^2 + 3\alpha + \frac{1}{2})z^2 + (\alpha^3 + 3\alpha^2 + \frac{3}{2}\alpha + \frac{1}{6})z^3}{(1+\alpha z)^3}. \tag{5.8}$$

It is third-order consistent; if α is given by (5.7b), then it is sixth-order dispersive, and fourth-order dispersive otherwise.

5.5. The case $m = 4$, $p = 3$. To achieve order of dispersion $q = 8$, the system

$$\begin{bmatrix} \gamma_0\alpha^4 - 6\gamma_2\alpha^2 + \gamma_4 & 4\alpha^3 + 6\gamma_0\alpha^2 - \gamma_2 & 4\alpha + \gamma_0 & 0 & 0 \\ -4\gamma_2\alpha^3 + 4\gamma_4\alpha & \alpha^4 + 4\gamma_0\alpha^3 - 4\gamma_2\alpha & 6\alpha^2 + 4\gamma_0\alpha & 1 & 0 \\ -\gamma_2\alpha^4 + 6\gamma_4\alpha^2 - \gamma_6 & \gamma_0\alpha^4 - 6\gamma_2\alpha^2 + \gamma_4 & 4\alpha^3 + 6\gamma_0\alpha^2 - \gamma_2 & 4\alpha + \gamma_0 & 0 \\ 4\gamma_4\alpha^3 - 4\gamma_6\alpha & -4\gamma_2\alpha^3 + 4\gamma_4\alpha & \alpha^4 + 4\gamma_0\alpha^3 - 4\gamma_2\alpha & 6\alpha^2 + 4\gamma_0\alpha & 1 \end{bmatrix} \begin{bmatrix} 1 \\ \frac{1}{2} \\ \hat{\beta}_4 \\ \tilde{\beta}_6 \\ \tilde{\beta}_8 \end{bmatrix} = \mathbf{0} \tag{5.9}$$

requires a real solution $(\alpha, \tilde{\boldsymbol{\beta}})$.

From the first and second equation, $\tilde{\beta}_4$ and $\tilde{\beta}_6$ are readily solved:

$$\tilde{\beta}_4 = -(\gamma_0\alpha^4 + 2\alpha^3 + (3\gamma_0 - 6\gamma_2)\alpha^2 + \gamma_4 - \tfrac{1}{2}\gamma_2)/(4\alpha + \gamma_0),$$

$$\tilde{\beta}_6 = \frac{\alpha^2}{4\alpha + \gamma_0}\left[6\gamma_0\alpha^4 + (10 + 4\gamma_0^2)\alpha^3 + \left(\frac{35}{2}\gamma_0 - 20\gamma_2\right)\alpha^2 + 10\gamma_0(\gamma_0 - 2\gamma_2)\alpha + 5\gamma_2 - 10\gamma_4\right].$$

On substitution into the third equation, and using the actual values for the γ's, we obtain an equation for the parameter α,

$$60\alpha^7 + 144\alpha^6 + 126\alpha^5 + 56\alpha^4 + 14\alpha^3 + 2\alpha^2 + \tfrac{16}{105}\alpha + \tfrac{1}{210} = 0,$$

possessing three real roots given by

$$\alpha^{(1)} = -.10058\,35034\cdots, \alpha^{(2)} = -.18716\,71826\cdots, \alpha^{(3)} = -1.12972\,65662\cdots. \tag{5.10}$$

Finally, $\tilde{\beta}_8$ follows from the last equation in (5.9) and the vector $\boldsymbol{\alpha}_4$ is determined by (4.4b). The stability function takes the form

$$R(z;\alpha) = \frac{1 + (4\alpha+1)z + (6\alpha^2 + 4\alpha + \frac{1}{2})z^2 + (4\alpha^3 + 6\alpha^2 + 2\alpha + \frac{1}{6})z^3 + (\alpha^4 + 4\alpha^3 + 3\alpha^2 + \frac{2}{3}\alpha + \tilde{\beta}_4)z^4}{(1+\alpha z)^4}. \tag{5.11}$$

This family furnishes sixth-order dispersive stability functions for all real α; in the particular case of (5.10) these functions are eighth-order dispersive.

6. Construction of third-order DIRK schemes. Let us start with an m-stage DIRK scheme, generated by the parameter matrix

$$
(6.1)\qquad
\begin{array}{c|cccccccc}
-\alpha & -\alpha & & & & & & & \\
c_2 & c_2+\alpha & -\alpha & & & & & & \\
c_3 & 0 & c_3+\alpha & -\alpha & & & & & \\
\vdots & \vdots & \ddots & \ddots & \ddots & & & & \\
c_{m-2} & \vdots & & \ddots & \ddots & \ddots & & & \\
c_{m-1} & 0 & \cdots & \cdots & 0 & c_{m-1}+\alpha & -\alpha & & \\
c_m & 0 & \cdots & \cdots & \cdots & 0 & c_m+\alpha & -\alpha & \\
\hline
 & 0 & \cdots & \cdots & \cdots & 0 & 1-b_m & b_m &
\end{array}.
$$

By this special choice, its implementation on a computer will require only a few arrays.

The parameters $c_2, \cdots, c_{m-2}$ will be used to adapt its stability function to the form required by the dispersion considerations (cf. § 5); α is prescribed and c_{m-1}, c_m and b_m will be required to satisfy the set of equations

$$(6.2a)\qquad (1-b_m)c_{m-1}+b_m c_m = \tfrac{1}{2},$$

$$(6.2b)\qquad (1-b_m)c_{m-1}^2+b_m c_m^2 = \tfrac{1}{3},$$

$$(6.2c)\qquad (1-b_m)[(c_{m-1}+\alpha)c_{m-2}-c_{m-1}\alpha]+b_m[(c_m+\alpha)c_{m-1}-c_m\alpha] = \tfrac{1}{6},$$

yielding third-order accuracy.

6.1. The case $m=3$. For a three-stage method, there are no free c-parameters left, because $c_{m-2}=c_1=-\alpha$. However, as any three-stage, third-order DIRK scheme (with α prescribed) has the same stability function (i.e., the function $R(z;\alpha)$, given by (5.8)), there is no need for any adaptation. Hence, solving (6.2) results automatically in a scheme that possesses the required stability function. From (6.2a) and (6.2b) we easily deduce

$$(6.3a)\qquad c_m = \frac{\frac{1}{3}-\frac{1}{2}c_{m-1}}{\frac{1}{2}-c_{m-1}},\qquad b_m = \frac{(\frac{1}{2}-c_{m-1})^2}{\frac{1}{3}-c_{m-1}+c_{m-1}^2},$$

and, on substitution, (6.2c) requires that c_{m-1} satisfy

$$(6.3b)\qquad 6c_{m-1}^3-9c_{m-1}^2+4c_{m-1}-\frac{\alpha(\alpha+2)+2/3}{2\alpha+1}=0.$$

Hence, for any value of α, we obtain at least one set of real parameters $\{c_{m-1}, c_m, b_m\}$.

For the special α-values given by (5.7b), this scheme is sixth-order dispersive. It turns out that for $\alpha=\alpha^{(2)}$, the stability function (5.8) is A-acceptable; that is, $R(z,\alpha^{(2)})$, which is a rational approximation to e^z, satisfies $|R(z,\alpha^{(2)})|<1$ whenever Re $z<0$ (cf. [9, p. 237]). On the contrary, $\alpha=\alpha^{(1)}$ leads to a conditionally stable scheme. Hence, for $m=3$, we will use $\alpha=\alpha^{(2)}$, yielding the scheme

$$
(6.4)\qquad
\begin{array}{c|ccc}
-\alpha & -\alpha & & \\
c_2 & c_2+\alpha & -\alpha & \\
c_3 & 0 & c_3+\alpha & -\alpha \\
\hline
 & 0 & 1-b_3 & b_3
\end{array}
\quad\text{with}\quad
\begin{array}{l}
\alpha \simeq -0.97567\,45887,\\
c_2 \simeq 0.11484\,20358,\\
c_3 \simeq 0.71636\,14441,\\
b_3 \simeq 0.64030\,84570.
\end{array}
$$

6.2. The case $m=4$. To construct a four-stage method, we again impose the order conditions (6.2), but now the resulting scheme does not automatically yield the stability function as given by (5.11). In general, the coefficient of z^4 in the numerator will be different. Therefore, we derived this coefficient for scheme $\{(6.1), m=4\}$ (cf. (2.6a)), and we identified the resulting expression with the corresponding expression in the required stability function (5.11). This equation, together with (6.2) was solved numerically for the unknowns c_2, c_3, c_4, and b_4. For all values of α, the resulting scheme is sixth-order dispersive. However, if we employ the special α-values given by (5.10), this order can be increased to eight. It turned out that only $\alpha^{(3)}$ yields an A-acceptable stability function, whereas $\alpha^{(1)}$ and $\alpha^{(2)}$ result in schemes with very poor stability characteristics, especially along the imaginary axis.

Hence, for $m=4$, we will use $\{(6.1), \alpha=\alpha^{(3)}\}$ leading to the scheme

$$(6.5)\qquad \begin{array}{c|cccc} -\alpha & -\alpha & & & \\ c_2 & c_2+\alpha & -\alpha & & \\ c_3 & 0 & c_3+\alpha & -\alpha & \\ c_4 & 0 & 0 & c_4+\alpha & -\alpha \\ \hline & 0 & 0 & 1-b_4 & b_4 \end{array} \quad \text{with} \quad \begin{array}{l} \alpha \simeq -1.12972\,65662, \\ c_2 \simeq 0.50160\,90786, \\ c_3 \simeq 0.72199\,89658, \\ c_4 \simeq 0.12462\,28759, \\ b_4 \simeq 0.37162\,34539. \end{array}$$

7. Numerical experiments. We have applied the methods (6.4) and (6.5), and the "conventional" methods

$$(7.1)\qquad \begin{array}{c|cc} -\alpha & -\alpha & \\ 1+\alpha & 1+2\alpha & -\alpha \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}, \qquad \alpha = -\left(\frac{1}{2}+\frac{1}{6}\sqrt{3}\right)$$

of Nørsett [10], and

$$(7.2)\qquad \begin{array}{c|ccc} \frac{1}{2}(1+\gamma) & \frac{1}{2}(1+\gamma) & & \\ \frac{1}{2} & -\frac{1}{2}\gamma & \frac{1}{2}(1+\gamma) & \\ \frac{1}{2}(1-\gamma) & 1+\gamma & -1-2\gamma & \frac{1}{2}(1+\gamma) \\ \hline & \frac{1}{6\gamma^2} & 1-\frac{1}{3\gamma^2} & \frac{1}{6\gamma^2} \end{array}, \qquad \gamma = \frac{2}{\sqrt{3}}\cos\left(\frac{\pi}{18}\right)$$

of Crouzeix [5] (see also Burrage [2]). All methods are A-stable; a further specification is given below:

Method	m	p	q	$\|R(\infty)\|$
(7.1)	2	3	4	0.732
(7.2)	3	4	4	0.630
(6.4)	3	3	6	0.679
(6.5)	4	3	8	0.655

Note that the methods of Nørsett and Crouzeix have optimal algebraic order, i.e., $p=m+1$.

In our numerical experiments, the accuracy was measured by the number of correct significant digits of the first component of the numerical solution at the endpoint $T=t_N$, i.e., the value of $sd := -\log_{10}|y^{(1)}(T)-y_N^{(1)}|$. If T coincides with a zero of $y^{(1)}(t)$, then this value can be used for a mutual comparison of the phase errors of the various methods (cf. [8]).

TABLE 7.1
Problem (7.3) *with* $\omega = 5$ *and* $T = 1001(\pi/2\omega)$.

Method	$h=\pi/16\omega$	$h=\pi/32\omega$	$h=\pi/64\omega$	$h=\pi/128\omega$	p_{eff}
(7.1)	1.1	1.9	3.1	4.3	4
(7.2)	0.6	1.7	2.8	4.0	4
(6.4)	2.1	3.6	5.3	7.1	6
(6.5)	3.0	5.1	7.5	9.9	8

7.1. A model problem. Consider the equation

$$\frac{dy}{dt} = \begin{bmatrix} 0 & \omega \\ -\omega & 0 \end{bmatrix} y, \qquad \omega \in \mathbb{R} \tag{7.3}$$

with initial condition $y(0) = (1, 0)^T$. The exact solution is given by

$$y = \begin{bmatrix} \cos(\omega t) \\ \sin(\omega t) \end{bmatrix}.$$

This problem belongs to the class of model problems to which the theory of the preceding sections applies. In Table 7.1 the $sd(h)$-values are presented for $\omega = 5$, $T = 1001(\pi/2\omega)$ and for various integration steps h. In addition, we list the effective order $p_{\text{eff}} := (sd(h) - sd(2h))/\log_{10}(2)$. These results show that the effective order is just the order of dispersion q as predicted by the theory.

7.2. A stiff problem with oscillating solution. In order to illustrate the A-stability of the various methods, we consider the problem

$$\frac{dy}{dt} = \begin{bmatrix} 113+1000t & 26+200t & -16-200t \\ -374-2500t & -86-500t & 53+500t \\ 191+3000t & 44+600t & -27-600t \end{bmatrix} y, \tag{7.4}$$
$$y(0) = (-1, 5, 1)^T;$$

the first component of the exact solution is given by

$$y^{(1)}(t) = \sin(t) - 3\cos(t) + 2\exp(-50t^2).$$

Evidently, this problem is highly stiff; the solution consists of undamped oscillating components and a rapidly decaying component (the stiff component).

In the numerical experiments, the initial phase was integrated using extremely small steps in order to avoid errors coming from the transient phase. From $t = 1$ on, the steps used are those listed in Table 7.2. The superiority of the methods with high dispersion order is again clear from these results.

TABLE 7.2
Problem (7.4) *with* $T = 10\pi + \arctan(3)$ *and* $h = (T-1)/N$.

Method	$N=50$	$N=100$	$N=200$	$N=400$	p_{eff}
(7.1)	0.2	1.1	2.2	3.4	4
(7.2)	1.1	1.0	2.1	3.2	~3.7
(6.4)	0.5	1.8	3.5	5.3	6
(6.5)	0.7	2.4	4.7	7.7	~9

7.3. The effect of changing frequencies. In the preceding problems the frequencies of the oscillating solution components did not depend on t. We now show the influence of a variable frequency on the accuracy of the numerical solution. For this purpose, we again consider problem (7.4). Let us denote the entries of the matrix occurring in (7.4) by $a_{i,j}+b_{i,j}t$. If these entries are replaced by

$$a_{i,j}(1+2\varepsilon t)+b_{i,j}t, \qquad \varepsilon \text{ constant}, \tag{7.5}$$

we obtain a problem, the solution of which no longer has a constant frequency. For instance,

$$y^{(1)}(t)=\sin(\omega t)-3\cos(\omega t)+2\exp(-50t^2),$$

where the frequency $\omega=1+\varepsilon t$. The analogue of Table 7.2 is given in Table 7.3 for $\varepsilon=10^{-2}$ and $\varepsilon=10^{-1}$. These results clearly show the drop in accuracy of the high-order dispersive methods (6.4) and (6.5), whereas the conventional methods (7.1) and (7.2) lose only a small amount of their *sd*-values. However, the higher-order dispersive methods are still superior to the conventional methods.

7.4. The effect of damped oscillations. Finally, we consider the behaviour of the high-order dispersive methods in problems with damped oscillations. As a test equation we take Bessel's equation

$$t^2\frac{d^2y}{dt^2}+t\frac{dy}{dt}+t^2y=0, \qquad 10\leqq t\leqq T \tag{7.6}$$

with the solution $y(t)=J_0(t)$.

By writing this second-order equation as a system of first-order equations we can apply the various DIRK methods.

Table 7.4 presents results for T equaling the hundredth zero of $J_0(t)$, i.e., $T=Z_{100}:=313.3742660775$. Although the high-order dispersive methods furnish more accurate

TABLE 7.3
Problem (7.5) with $T=[10\pi+\arctan(3)]/(1+\varepsilon T)$ and $h=(T-1)/N$.

Method	ε	$N=50$	$N=100$	$N=200$	$N=400$	p_{eff}
(7.1)	10^{-2}	0.2	1.0	2.2	3.4	4
(7.2)	10^{-2}	1.4	1.0	2.0	3.2	4
(6.4)	10^{-2}	0.4	1.7	3.2	4.5	~4.5
(6.5)	10^{-2}	0.6	2.1	3.3	4.2	~3.5
(7.1)	10^{-1}	0.1	0.9	2.0	3.1	~3.7
(7.2)	10^{-1}	0.8	0.9	1.8	2.9	~3.5
(6.4)	10^{-1}	0.3	1.4	2.8	4.1	~4.5
(6.5)	10^{-1}	0.4	1.7	2.9	3.7	~3.5

TABLE 7.4
Problem (7.6) with $T=Z_{100}$ and $h=(T-10)/N$.

Method	$N=1000$	$N=2000$	$N=4000$	$N=8000$	P_{eff}
(7.1)	2.3	3.2	4.3	5.4	~3.5
(7.2)	2.1	3.0	4.2	5.3	~4
(6.4)	2.9	4.1	5.1	6.0	~3
(6.5)	3.3	4.3	5.2	6.1	3

results than the methods of Nørsett and Crouzeix, they do not show the order of dispersion q, but instead, their algebraic order p. The reason is, of course, the $1/\sqrt{t}$-behaviour of the amplitude of the solution $y(t)$ (recall that $J_0(t) \sim$ constant $\cdot \cos(t-\pi/4)t^{-1/2}$ as $t \to \infty$). In order to illustrate this we transform (7.6) in such a way that the transformed equation has an undamped solution. Writing $t = 10\tilde{t}$ and $y(t) = \sqrt{10t}\,\tilde{y}(\tilde{t})$, we obtain

$$\frac{d^2\tilde{y}}{d\tilde{t}^2} + \left(100 + \frac{1}{4\tilde{t}^2}\right)\tilde{y} = 0, \qquad 1 \leqq \tilde{t} \leqq \frac{T}{10} \tag{7.6'}$$

with the undamped solution $\tilde{y}(\tilde{t}) = \sqrt{\tilde{t}}\, J_0(10\tilde{t})$. For this problem the results listed in Table 7.4′ do show the order of dispersion q rather nicely.

TABLE 7.4′
Problem (7.6′) *with* $T = Z_{100}$ *and* $h = (T-10)/(10N)$.

Method	$N=1000$	$N=2000$	$N=4000$	$N=8000$	p_{eff}
(7.1)	1.5	2.5	3.6	4.8	4
(7.2)	1.3	2.2	3.4	4.6	4
(6.4)	2.2	3.8	5.5	7.3	6
(6.5)	2.8	4.9	7.4	8.7	8

Acknowledgments. We are grateful to the referees for their careful reading of the manuscript and constructive remarks.

REFERENCES

[1] L. BRUSA AND L. NIGRO, *A one-step method for direct integration of structural dynamic equations*, Internat. J. Numer. Methods Engrg. 15 (1980), pp. 685-699.

[2] K. BURRAGE, *Efficiently implementable algebraically stable Runge-Kutta methods*, SIAM J. Numer. Anal., 19 (1982), pp. 245-258.

[3] M. M. CHAWLA AND P. S. RAO, *A Noumerov-type method with minimal phase-lag for the integration of second order periodic initial-value problems* II. *Explicit method*, J. Comput. Appl. Math., 15 (1986), pp. 329-337.

[4] M. M. CHAWLA, P. S. RAO, AND BENY NETA, *Two-step fourth-order P-stable methods with phase-lag of order six for* $y''=f(t,y)$, J. Comput. Appl. Math., 16 (1986), pp. 233-236.

[5] M. CROUZEIX, *Sur la B-stabilité des méthodes de Runge-Kutta*, Numer. Math., 32 (1979), pp. 75-82.

[6] K. DEKKER AND J. G. VERWER, *Stability of Runge-Kutta Methods for Stiff Nonlinear Differential Equations*, North-Holland, Amsterdam, New York, Oxford, 1984.

[7] I. GLADWELL AND R. M. THOMAS, *Damping and phase analysis of some methods for solving second order ordinary differential equations*, Internat. J. Numer. Methods Engrg. 19 (1983), pp. 495-503.

[8] P. J. VAN DER HOUWEN AND B. P. SOMMEIJER, *Explicit Runge-Kutta (-Nyström) methods with reduced phase errors for computing oscillating solutions*, SIAM J. Numer. Anal., 24 (1987), pp. 595-617.

[9] J. D. LAMBERT, *Computational Methods in Ordinary Differential Equations*, John Wiley, New York, London, 1973.

[10] S. P. NØRSETT, *Semi-explicit Runge-Kutta methods*, Report No. 6/74, University of Trondheim, Trondheim, Norway, 1974.

[11] H. J. STETTER, *Analysis of Discretization Methods for Ordinary Differential Equations*, Springer-Verlag, Berlin, Heidelberg, New York, 1973.

[12] E. STIEFEL AND D. G. BETTIS, *Stabilization of Cowell's method*, Numer. Math., 13 (1969), pp. 154-175.

[13] K. STREHMEL AND R. WEINER, *Nichtlineare Stabilität und Phasenuntersuchung adaptiver Nyström-Runge-Kutta Methoden*, Computing, 35 (1985), pp. 325-344.

[14] K. STREHMEL, *Stabilitäts- und Phasenuntersuchung von linear-impliziten Methoden für $y'' = f(t, y)$*, in Proc. 4e Tagung Numerische Behandlung von gewöhnliche Differentialgleichungen, R. März ed., Berlin, 1984.
[15] R. M. THOMAS, *Phase properties of high order, almost P-stable formulae*, BIT, 24 (1984), pp. 225–238.
[16] E. H. TWIZELL AND A. Q. M. KHALIQ, *Multiderivative methods for periodic initial value problems*, SIAM J. Numer. Anal., 21 (1984), pp. 111–122.