DIAGONALLY IMPLICIT RUNGE-KUTTA-NYSTRÖM METHODS FOR OSCILLATORY PROBLEMS*

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Abstract. Implicit Runge-Kutta-Nyström (RKN) methods are constructed for the integration of second-order differential equations possessing an oscillatory solution. Based on a linear homogeneous test model we analyse the *phase errors* (or *dispersion*) introduced by these methods and derive so-called dispersion relations. *Diagonally* implicit RKN methods of relatively low algebraic order are constructed, which have a high order of dispersion (up to 10). Application of these methods to a number of test examples (linear as well as nonlinear) yields a greatly reduced phase error when compared with "conventional" DIRKN methods.

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

AMS(MOS) subject classification. 65L05

1. Introduction. This paper extends the phase-lag (or dispersion) analysis of Runge-Kutta methods [12] and explicit Runge-Kutta-Nyström (RKN) methods [9] to diagonally implicit RKN (DIRKN) methods. The methods proposed here are devised for the accurate integration of the initial value problem

(1.1)
$$\ddot{y} = f(t, y), \quad y(0) = y_0, \quad \dot{y}(0) = \dot{y}_0,$$

where it is known that y(t) is dominated by oscillating solution components with slowly varying frequencies.

The approach for constructing such methods parallels the approach followed in [9] and [12]. First, we derive the dispersion relations in terms of the RKN parameters (see \S 2). Next, functions S and P characterizing the RKN method and satisfying the dispersion relations are constructed (\S 3). Finally, on the basis of these functions S and P, some RKN methods are computed (\S 4) yielding small dispersion errors.

We present a number of second-order two- and three-stage methods with dispersion orders four to ten. These methods are compared with a "conventional" DIRKN method of order four using two stages, which requires a comparable computational effort. In § 5, the methods are applied to a set of test problems, both linear and nonlinear examples. The new methods behave markedly more accurately than the conventional method (for example, a reduction of the phase-lag error by a factor 1000 is not exceptional). It turns out that these large reduction factors are also obtained for the nonlinear problems, although these nonlinear oscillators differ considerably from the linear model problem on which the theory is based.

We note that recently a large number of papers have been published proposing methods with high-order phase-lag. A few of them deal with first-order differential equations [1], [9], and [12], but the majority are devoted to the second-order case. In Gladwell and Thomas [7] linear multistep (LM) methods are considered. However, it is well known [14] that the order of such methods is restricted to two, if *P*-stability (see § 3.1) is required. To overcome this barrier, Cash [2], Thomas [18], and Chawla et al. [3], [4] have considered hybrid variants of these LM methods, by introducing offstep points in the formulae to obtain methods that fit into the class of general multistep Runge-Kutta methods. Within this class it is possible to achieve high-order

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P-stable methods. In connection with this, we also mention the papers of Hairer [8] and Kambo, Jain, and Goel [13]. Rosenbrock-type methods (adaptive RKN methods) are considered by Strehmel [16] and Strehmel and Weiner [17]; here, the phase-lag analysis is restricted to the effects of inhomogeneous terms. The extension of this analysis to explicit RKN methods and predictor-corrector (PC) methods is described in [11]. Furthermore, we mention the work of Twizell [21] and Twizell and Khaliq [20], who have investigated multiderivative methods, and the PC-type methods that have been studied by van der Houwen and Sommeijer [10].

Most of the above-mentioned methods are implicit and thus require the solution of an algebraic equation in each step. Here, we are faced with a nontrivial task: for the fully implicit RKN methods it is well known that the dimension of the system to be solved is a multiple of the dimension of the ODE. The hybrid methods, viewed as RKN methods, exhibit the same difficulty. However, this class of methods can also be implemented in such a way that the dimension of the system is not increased. On the other hand, if some form of Newton iteration is used, powers of the Jacobian matrix $(\partial f/\partial y)$ enter into the solution process, i.e., systems of the form

$$\left[I - \gamma_1 h^2 \left(\frac{\partial f}{\partial y}\right) - \gamma_2 h^4 \left(\frac{\partial f}{\partial y}\right)^2 - \cdots\right] \Delta y = \Sigma$$

must be solved. Obviously, this is unattractive from a computational point of view. One way to overcome this is to factor the matrix into a product of matrices. The coefficients in these matrices should be real, however, which in turn restricts the attainable order. For an extensive discussion on this subject, refer to [2], [18].

Furthermore, it is clear that the multiderivative approach may also lead to serious computational problems because, as in many practical problems, the explicit calculation of these higher derivatives is excessively laborious.

Moreover, the multistep methods need a starting procedure and, as Cash [2] pointed out, this is a nontrivial problem.

Therefore, we think that the DIRKN methods described in this paper may offer a useful alternative if *P*-stability in combination with a high (phase-lag) order is required; they are of one-step nature (i.e., self-starting) and, due to the diagonally implicit structure, they allow for a very efficient implementation.

2. Dispersion and dissipation in RKN methods. The general m-stage RKN method for the system of ODEs (1.1) is given by

$$Y_{nj} = y_n + c_j h \dot{y}_n + h^2 \sum_{l=1}^m a_{jl} f(t_n + c_l h, Y_{nl}), \qquad j = 1, \dots, m,$$

$$(2.1) \qquad y_{n+1} = y_n + h \dot{y}_n + h^2 \sum_{j=1}^m b_j f(t_n + c_j h, Y_{nj}),$$

$$\dot{y}_{n+1} = \dot{y}_n + h \sum_{j=1}^m b'_j f(t_n + c_j h, Y_{nj}),$$

where the RKN parameters a_{jl} , b_j , b'_j , and c_j are assumed to be real. By defining

$$(2.2) A := (a_{ji}), \quad \mathbf{b} := (b_j), \quad \mathbf{b}' := (b'_j), \quad \mathbf{c} := (c_j),$$

the RKN method can be represented by the Butcher array:

$$\begin{array}{c|c}
\mathbf{c} & A \\
\hline
 & \mathbf{b}^T \\
\hline
 & \mathbf{b}^{\prime T}
\end{array}$$

2.1. Homogeneous test equation. In this section we consider the homogeneous test equation

$$(2.3) \ddot{y} = -\omega^2 y, \omega \in \mathbb{R},$$

which will also be referred to as the *model problem*. On the basis of this model problem, we will derive the conditions for RKN methods to possess a small dispersion error. In § 5, we will show, by some nonlinear examples, that the obtained results apply to a large extent also in the *nonmodel* situation.

Application of (2.1) yields the recursion

(2.4a)
$$y_{n+1} = y_n + h\dot{y}_n - v^2\mathbf{b}^T\mathbf{Y}_n, \qquad h\dot{y}_{n+1} = h\dot{y}_n - v^2\mathbf{b}^{T}\mathbf{Y}_n,$$

where

$$(2.4b) v := \omega h, \quad \mathbf{Y}_n := N^{-1}(y_n \mathbf{e} + h \dot{y}_n \mathbf{c}), \quad N := I + v^2 A, \quad \mathbf{e} = (1, \dots, 1)^T.$$

Elimination of the auxiliary vector Y_n yields

(2.5)
$$\begin{pmatrix} y_{n+1} \\ h\dot{y}_{n+1} \end{pmatrix} = M(v^2) \begin{pmatrix} y_n \\ h\dot{y}_n \end{pmatrix}, \qquad M(v^2) := \begin{pmatrix} 1 - v^2 \mathbf{b}^T N^{-1} \mathbf{e} & 1 - v^2 \mathbf{b}^T N^{-1} \mathbf{c} \\ -v^2 \mathbf{b}'^T N^{-1} \mathbf{e} & 1 - v^2 \mathbf{b}'^T N^{-1} \mathbf{c} \end{pmatrix}.$$

Following [9] we introduce the functions

(2.6)
$$S(v^2) := \operatorname{Trace}(M), \quad P(v^2) := \operatorname{Det}(M),$$

and we define the phase error or dispersion of the RKN method by

(2.7)
$$\phi(v) := v - \arccos\left[\frac{S(v^2)}{2\sqrt{P(v^2)}}\right]$$

and the amplification error or dissipation by

(2.8)
$$\alpha(v) := 1 - \sqrt{P(v^2)};$$

here, it is assumed that $M(v^2)$ has complex conjugate eigenvalues for sufficiently small values of v.

Let us write the exact solution of (2.3) in the form

$$y(t_n) = y(nh) = c \cos(\psi + nv),$$

where c and ψ are real constants determined by the initial conditions; a similar expression holds for the numerical solution:

$$y_n = \tilde{c}(1 - \alpha(v))^n \cos{(\tilde{\psi} + nv - n\phi(v))},$$

where \tilde{c} and $\tilde{\psi}$ are real constants determined by y_0 and \dot{y}_0 , and the RKN parameters (see [9]).

These expressions show that the dispersion and dissipation errors $\phi(v)$ and $\alpha(v)$ are accumulated in the numerical integration process. In the case of long interval integrations these errors may give rise to considerable numerical errors. Therefore, it is of interest to construct RKN methods for which $\phi(v)$ and $\alpha(v)$ are of high orders in v as v (i.e., h) tends to zero. In this paper we concentrate on the derivation of methods that have a high order of dispersion. In addition, some of the methods to be derived have zero dissipation, i.e., $\alpha(v) \equiv 0$. As a consequence, when applying these methods, the numerical errors produced are often mainly determined by $\psi - \tilde{\psi}$ and $c - \tilde{c}$. These errors were respectively termed *initial dispersion* and *initial dissipation* in [9]. In our numerical experiments we shall use a test strategy that eliminates these initial errors from the numerical error estimated.

2.2. Dispersion relations. Let us start by deriving the *local truncation error* of the RKN method for the test equation (2.3). Elimination of \dot{y}_n from (2.5) yields the recursion

$$(2.5') y_{n+1} - S(v^2)y_n + P(v^2)y_{n-1} = 0;$$

hence, the local truncation error $\tau(v)$ of this linear two-step method is defined by substitution of the exact solution of (2.3) into (2.5'):

(2.9)
$$\tau(v) := e^{2iv} - S(v^2) e^{iv} + P(v^2).$$

If the RKN method is of (algebraic) order p then

(2.10)
$$\tau(v) = O(v^{p+2}).$$

We will likewise call the RKN method dispersive and dissipative of orders q and r, if, respectively,

(2.11)
$$\phi(v) = O(v^{q+1}), \qquad \alpha(v) = O(v^{r+1}).$$

It should be remarked that (2.11) is a sufficient and necessary condition for a qth order dispersive, rth order dissipative method, whereas (2.10) is only a *necessary* condition for algebraic order p.

It is convenient to introduce the notions of consistent, dispersive, and dissipative functions S and P, and the concept of P-stability.

DEFINITION 2.1. The functions $S(v^2)$ and $P(v^2)$ are called *consistent*, dispersive, and dissipative of orders p, q, and r, respectively, if (2.10) and (2.11) are satisfied. The RKN method is called P-stable (or unconditionally zero dissipative) if $P(v^2) \equiv 1$ and $|S(v^2)| < 2$ for all $v^2 > 0$.

P-stability was introduced by Lambert and Watson [14] for linear multistep methods and extended to other numerical methods by Hairer [8].

The following theorem summarizes a few properties of the functions S and P which are straightforwardly proved.

THEOREM 2.1. (a) The functions $S(v^2)$ and $P(v^2)$ are consistent, dispersive and dissipative of orders p, q, and r, if, respectively,

$$\begin{split} &e^{iv}[2\cos{(v)} - S(v^2)] + P(v^2) - 1 = O(v^{p+2}), \\ &S(v^2) - 2\sqrt{P(v^2)}\cos{(v)} = O(v^{q+2}), \\ &P(v^2) - 1 = O(v^{r+1}). \end{split}$$

- (b) An RKN method of algebraic order p, dispersion order q, and dissipation order r possesses functions S and P that are consistent, dispersive, and dissipative of orders p, q, and r.
- (c) If S and P are dispersive and dissipative of orders q and r, then the corresponding RKN method is dispersive and dissipative of orders q and r.
- (d) An RKN method of algebraic order p is dispersive and dissipative of orders $q \ge 2 \lfloor (p+1)2 \rfloor$ and $r \ge 2 \lfloor (p+1)/2 \rfloor$.
- (e) If $P(v^2) \equiv 1$ then the orders of consistency and dispersion of S and P are equal. To facilitate the construction of high-order dispersive functions S and P, we introduce the Taylor expansions of S and P:

(2.12)
$$S(z) = 2 - \sigma_1 z + \sigma_2 z^2 - \sigma_3 z^3 + \cdots$$
, $P(z) = 1 - \pi_1 z + \pi_2 z^2 - \pi_3 z^3 + \cdots$,

and we express the order conditions (2.10) and (2.11) directly in terms of the coefficients σ_j and π_j . The dispersion and consistency relations are easily derived from Tables 2.1 and 2.2. We note that in the context of *explicit* RKN methods the dispersion relations have already been derived in [9].

TABLE 2.1
$$\phi(v) = \sum_{j=1}^{\infty} F_{2j} v^{2j-1}$$
.

$$\begin{split} F_2 &= -[\sigma_1 - \pi_1 - 1] \\ F_4 &= [\sigma_1^2 + 4\sigma_2 - 4\pi_1 - 4\pi_2 - \frac{4}{3}]/8 \\ F_6 &= -[6\sigma_1\sigma_2 + 12\sigma_3 - 4\pi_1 - 12\pi_2 - 12\pi_3 - \frac{8}{15}]/24 \\ F_8 &= [45\sigma_2^2 + 90\sigma_1\sigma_3 + 180\sigma_4 - 8\pi_1 - 60\pi_2 - 180\pi_3 - 180\pi_4 - \frac{4}{7}]/360 \\ F_{10} &= -[45\sigma_2\sigma_3 + 45\sigma_1\sigma_4 + 90\sigma_5 - 2\pi_1/7 - 4\pi_2 - 30\pi_3 - 90\pi_4 - 90\pi_5 - \frac{4}{315}]/180 \\ F_{12} &= [315\sigma_3^2 + 1260\sigma_6 + 630\sigma_1\sigma_5 + 630\sigma_2\sigma_4 - 8\pi_1/45 - 4\pi_2 - 56\pi_3 - 420\pi_4 - 1260\pi_5 - 1260\pi_6 - \frac{8}{1485}]/2520 \\ \end{split}$$

TABLE 2.2
$$\tau(v) = \sum_{j=2}^{\infty} T_j v^j.$$

$$T_2 = \sigma_1 - \pi_1 - 1$$

$$T_3 = i(\sigma_1 - 1)$$

$$T_4 = -\frac{1}{2}\sigma_1 - \sigma_2 + \pi_2 + \frac{7}{12}$$

$$T_5 = -i\left[\frac{1}{6}\sigma_1 + \sigma_2 - \frac{1}{4}\right]$$

$$T_6 = \frac{1}{24}\sigma_1 + \frac{1}{2}\sigma_2 + \sigma_3 - \pi_3 - \frac{31}{360}$$

The coefficients σ_j are easily expressed in terms of the RKN parameters. It follows from (2.6) that

$$(2.13) S(z) = 2 - z [\mathbf{b}^T N^{-1} \mathbf{e} + \mathbf{b}'^T N^{-1} \mathbf{c}], z := v^2.$$

On substitution of $N = I + v^2 A = I + zA$ and expanding N^{-1} in a Taylor series, we readily obtain

(2.14)
$$\sigma_i = \mathbf{b}^T A^{j-1} \mathbf{e} + \mathbf{b}'^T A^{j-1} \mathbf{c}.$$

In general, the coefficients π_j are much more complicated expressions in terms of the RKN parameters. However, in the particular case where we have $\mathbf{b}' = \beta \mathbf{b}$ or $\mathbf{c} = \gamma \mathbf{e}$, with β and γ scalars, we obtain

(2.15)
$$P(z) = 1 - z[\mathbf{b}^{T} N^{-1} \mathbf{e} + \mathbf{b}'^{T} N^{-1} \mathbf{c} - \mathbf{b}'^{T} N^{-1} \mathbf{e}],$$
$$= S(z) - 1 + z \mathbf{b}'^{T} N^{-1} \mathbf{e}$$

so that

(2.16)
$$\pi_{i} = \mathbf{b}^{T} A^{j-1} \mathbf{e} + \mathbf{b}'^{T} A^{j-1} (\mathbf{c} - \mathbf{e}) = \sigma_{i} - \mathbf{b}'^{T} A^{j-1} \mathbf{e}.$$

We note that the simplifying condition $\mathbf{b}' = \beta \mathbf{b}$ or $\mathbf{c} = \gamma \mathbf{e}$ restricts the algebraic order of the RKN method to one and two (this can be explained by observing that the algebraic order conditions for third-order consistency are expressed only in terms of \mathbf{b} , \mathbf{b}' , and \mathbf{c} , and do not allow the simplifying conditions).

2.3. Inhomogeneous test equation. The inhomogeneous test equation

(2.17)
$$\ddot{y} = -\omega^2 y + c \exp(i\omega_t t), \quad \omega, \omega_t \in \mathbb{R}, \quad \omega \neq \omega_t$$

is frequently used to model forced oscillations (see [7], [11], and [17]). Application

of the RKN method (2.1) yields the inhomogeneous recursion

where the matrix $M(v^2)$ is defined in (2.5) and

(2.19)
$$\mathbf{g} := \begin{pmatrix} \mathbf{b}^T N^{-1} \mathbf{e}_f \\ \mathbf{b}^T N^{-1} \mathbf{e}_f \end{pmatrix}, \quad \mathbf{e}_f := (\exp(iv_j c_l)), \quad v_f := h\omega_f.$$

It is easily verified that

satisfies the recursion (2.18). Hence, the *general* solution of the recursion (2.18) is composed of the *forced* solution component (2.20) and the general solution of the *homogeneous* recursion (2.5).

It is of interest to compare the forced solution component of the numerical solution with that of the exact solution, i.e., the component

It follows from (2.20) and (2.21) that the phase error and the dissipation error of the forced solution component do not depend on t_n , so that, contrary to $\phi(v)$ and $\alpha(v)$, they are not accumulated in time. Thus, also for the nonhomogeneous problem (2.17), it is the dispersion error $\phi(v)$ and the dissipation error $\alpha(v)$ that form the main source of inaccuracies when long interval integrations are performed.

3. Construction of functions S and P. From now on we shall confine our considerations to diagonally implicit m-stage RKN methods (DIRKN methods), i.e., the matrix A is lower triangular and $a_{ij} = a$ for $j = 1, \dots, m$. For such methods, S(z) assumes the form

(3.1)
$$S(z) = \frac{2 + \sigma_1^* z + \dots + \sigma_m^* z^m}{(1 + az)^m}.$$

In the following it will be assumed that P(z) has a similar form:

(3.2)
$$P(z) = \frac{1 + \pi_1^* z + \dots + \pi_m^* z^m}{(1 + az)^m}.$$

For instance, this happens when the simplifying condition $\mathbf{b}' = \beta \mathbf{b}$ or $\mathbf{c} = \gamma \mathbf{e}$ is satisfied (see (2.15)).

The functions S and P of the special form (3.1) and (3.2), and being consistent and dispersive of orders p and q, will be denoted by $S_m^{(p,q)}$ and $P_m^{(p,q)}$.

3.1. Zero-dissipative methods. In this section it is assumed that $P(z) \equiv 1$; for sufficiently small values of $z = v^2 = \omega^2 h^2$ this condition guarantees zero dissipation for any consistent RKN method. Such methods are said to have an *interval of periodicity* (cf. Lambert and Watson [14]).

In Table 3.1 we list a few functions $S_m^{(p,q)}$ obtained by solving the dispersion relations of Table 2.1 and by equating the coefficients in (2.12) and in the Taylor expansion of (3.1). (Note that, by virtue of Theorem 2.1(e), p = q.)

TABLE 3.1 Functions $S_m^{(p,q)}(z)$ of high dispersion order for DIRKN methods possessing an interval of periodicity $(0, H_0^2)$, i.e., $P(z) \equiv 1$.

$$\begin{split} m=1: & S_{1}^{(2,2)}(z) = \frac{2+(2a-1)z}{1+az}; \\ a & \geq \frac{1}{4} \\ a & = \frac{1}{12} \\ \end{split} \qquad \Rightarrow q=2, \quad H_{0}^{2} = \infty \\ a & = \frac{1}{12} \\ \end{split} \qquad \Rightarrow q=4, \quad H_{0}^{2} = 6 \\ \\ m=2: & S_{2}^{(4,4)}(z) = \frac{2+(4a-1)z+(2a^{2}-2a+\frac{1}{12})z^{2}}{(1+az)^{2}}; \\ a & > \frac{1}{4} + \frac{\sqrt{6}}{12} \\ a & = \frac{1}{12} + \frac{\sqrt{15}}{60} \\ a & = \frac{1}{12} - \frac{\sqrt{15}}{60} \\ \Rightarrow q=6, \quad H_{0}^{2} = 6.43 \\ a & = \frac{1}{12} - \frac{\sqrt{15}}{60} \\ \Rightarrow q=6, \quad H_{0}^{2} \approx 21.85 \\ \end{split}$$

$$m=3: & S_{3}^{(6,6)}(z) = \frac{2+(6a-1)z+(6a^{2}-3a+\frac{1}{12})z^{2}+(2a^{3}-3a^{2}+\frac{1}{4}a-\frac{1}{360})z^{3}}{(1+az)^{3}}; \\ a & > 0.656 \cdot \cdots \\ a & = a^{(1)} = 0.2117520482855 \\ \Rightarrow q=6, \quad H_{0}^{2} = \infty \\ a & = a^{(1)} = 0.217520482855 \\ \Rightarrow q=8, \quad H_{0}^{2} \approx 6.64 \\ a & = a^{(2)} = 0.7657710662139_{10} \\ \Rightarrow q=8, \quad H_{0}^{2} \approx 9.33 \\ a & = a^{(3)} = 0.3059024105236_{10} \\ \end{array} \qquad \Rightarrow q=8, \quad H_{0}^{2} \approx 24.15 \end{split}$$

We also list the interval of periodicity defined by

$$(3.3) (0, H_0^2) := \{z | z > 0, P(z) \equiv 1, |S(z)| < 2\}.$$

3.2. Dissipative methods. When second-order hyperbolic equations are solved by means of the method of lines it is advisable to use time integrators that damp the high time frequencies in the solution. In other words, if RKN methods are used, the method should be dissipative in the sense that the eigenvalues of the amplification matrix M are within the unit circle. Therefore, we drop the condition $P(z) \equiv 1$ of the preceding section. Consequently, there is no longer an interval of periodicity, but an interval of strong stability defined by

$$(3.4) (0, \beta^2) := \{z | z > 0, P(z) < 1, |S(z)| < P(z) + 1\}.$$

In Table 3.2 a few high-order dispersive pairs $\{S, P\}$ are given together with the stability interval $(0, \beta^2)$. We observe that the functions $\{S_1^{(3,4)}, P_1^{(3,4)}\}$ are identical to the one-stage functions $\{S_1^{(4,4)}, P_1^{(4,4)} \equiv 1\}$ of the preceding section. Furthermore, there exists no unconditionally stable pair $\{S_2^{(2,6)}, P_2^{(2,6)}\}$; the largest interval of (weak) stability is obtained for $a = 1/12 - \sqrt{15}/60$ and leads to the two-stage zero-dissipative functions of Table 3.1.

4. Construction of DIRKN methods of high dispersion order. The construction of DIRKN methods yielding small dispersion errors consists of the identification of the S and P functions of a given class of methods with one of the function pairs given in § 3. The following lemma is helpful (cf. [12]) for finding a convenient expression for S and P.

LEMMA 4.1. Let N be a nonsingular m by m matrix, and let v and w be m-dimensional vectors. Then

$$\mathbf{v}^T N^{-1} \mathbf{w} = \frac{\text{Det} [N + \mathbf{w} \mathbf{v}^T]}{\text{Det} [N]} - 1.$$

TABLE 3.2

Functions $S_m^{(p,q)}(z)$ and $P_m^{(p,q)}(z)$ of high dispersion order for DIRKN methods possessing an interval of (strong) stability $(0, \beta^2)$.

$$m=1: \qquad S_1^{(1,q)}(z) = \frac{2+\sigma_1^*z}{1+az}, \quad P_1^{(1,q)}(z) = \frac{1+(1-a+\sigma_1^*)z}{1+az}, \quad q \geq 2.$$

$$(i) \quad -\frac{1}{2} \leq \sigma_1^* < 2a - 1, \quad a > 0 \Rightarrow q = 2, \quad \beta^2 = \infty$$

$$(ii) \quad \sigma_1^* = 2 \left[a - 1 - \sqrt{\frac{1}{3}} - a \right], \quad a \leq \frac{1}{3} (a \neq 0) \Rightarrow q = 4, \quad \beta^2 = \min \left(\frac{-4}{2\sigma_1^*+1}, \begin{cases} \infty & \text{if } a > 0 \\ -1/a, & a < 0 \end{cases} \right)$$

$$(iii) \quad \sigma_1^* = 2 \left[a - 1 + \sqrt{\frac{1}{3}} - a \right], \quad \frac{1}{12} < a \leq \frac{1}{3} \Rightarrow q = 4, \quad \beta^2 = \frac{-4}{2\sigma_1^*+1}$$

$$m = 2: \qquad S_2^{(3,q)}(z) = \frac{2 + (4a - 1) + (\pi_2^* + a^2 - 2a + \frac{1}{12})z^2}{(1+az)^2}, \qquad q \geq 4.$$

$$(i) \quad -a^2 + a - \frac{1}{24} \leq \pi_2^* < a^2, \quad a \geq \frac{1}{8} \Rightarrow q = 4, \quad \beta^2 = \infty$$

$$(ii) \quad \pi_2^* = -a^2 + \frac{a}{3} - \frac{1}{180} \Rightarrow q = 6$$

$$a > \frac{1}{12} + \frac{1}{60} \sqrt{15} \Rightarrow \beta^2 = A \left[1 + \sqrt{1 - \frac{8}{A(1-8a)}} \right], \quad A = \frac{90(1-8a)}{(13-240a)}$$

$$a < \frac{1}{12} - \frac{1}{60} \sqrt{15} \Rightarrow \beta^2 = \frac{12}{(1-24a)}$$
For all other values of a we have $\beta^2 = 0$

$$(iii) \quad \pi_2^* = -a^2 + \frac{a}{3} - \frac{1}{180}$$

$$\sigma_2(3\sigma_2 - 12a - 4) - a(24a^2 + 3a - 2) + \frac{31}{105} = 0$$

$$\Rightarrow q = 8$$

$$\sigma_2 = \frac{7}{90} + \frac{a}{3} - 2a^2$$

$$a = 0.3148024587598 \Rightarrow q = 8, \quad \beta^2 = 6.21$$

$$a = 0.0218432425854 \Rightarrow q = 8, \quad \beta^2 = 6.21$$

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By means of this lemma the inverse of the matrix $N = I + v^2 A$ occurring in the matrix $M(v^2)$ can be eliminated so that $S(v^2)$ and $P(v^2)$ as defined in (2.6) are easier to evaluate.

4.1. A one-stage method of algebraic order p=2. Consider the second-order, one-parameter family of DIRKN methods generated by the Butcher array:

The corresponding functions S and P are given by

$$S(z) = \frac{2 + (2a - 1)z}{1 + az}, \qquad P(z) \equiv 1.$$

For $a = \frac{1}{12}$ the function S(z) is identical with the function $S_1^{(4,4)}(z)$ of Table 3.1, so that (4.1) is fourth-order dispersive for $a = \frac{1}{12}$ with periodicity interval (0,6).

4.2. Two-stage methods of algebraic order p = 2. We start with the three-parameter family of algebraic order two:

$$\begin{array}{c|ccccc}
c & a \\
\frac{1}{2} & a_1 & a \\
\hline
0 & \frac{1}{2} \\
0 & 1
\end{array}$$

We find the functions

$$S(z) = \frac{2 + (4a - 1)z + (2a^2 - a + a_1/2 + ca_1)z^2}{(1 + az)^2},$$

$$P(z) = \frac{1 + 2az + (a^2 - a_1/2 + ca_1)z^2}{(1 + az)^2}.$$

If we choose $c=\frac{1}{2}$ and $a_1=\frac{1}{12}-a$, we have $P(z)\equiv 1$ and $S(z)\equiv S_2^{(4,4)}(z)$ as given in Table 3.1. We mention two particular methods: the sixth-order dispersive method:

with periodicity interval (0, 21.85) and the fourth-order dispersive, P-stable method:

Identification with the functions $S_2^{(3,6)}(z)$ and $P_2^{(3,6)}(z)$ is obtained for $a_1 = \frac{1}{12} - a$, $c = (24a^2 + 2a - \frac{13}{30})/(12a - 1)$ leading to a one-parameter family of sixth-order dispersive, dissipative methods generated by

$$(4.5) \qquad \begin{array}{c|c} (24a^2 + 2a - \frac{13}{30})/(12a - 1) & a \\ \frac{\frac{1}{2}}{0} & \frac{\frac{1}{12} - a - a}{0} \\ 0 & \frac{1}{2}. \end{array}$$

Eighth-order dispersion is obtained for a = 0.3148024587598 with strong stability interval (0, 6.21).

Finally, identification with the functions $S_2^{(3,4)}(z)$ and $P_2^{(3,4)}(z)$ with $\pi_2^* = 0$ of Table 3.2 leads to the fourth-order dispersive methods:

$$(4.6) \qquad \begin{array}{c|c} (12a^2 + 6a - \frac{1}{2})/(12a - 1) & a \\ \frac{\frac{1}{2}}{2} & \frac{\frac{1}{12} - a - a}{0 - \frac{1}{2}}, \\ 0 & 1 \end{array}$$

which are unconditionally strongly stable for $a \ge \frac{1}{2} + \frac{\sqrt{30}}{12}$. In the numerical experiments we will use a = 1.

4.3. Two three-stage methods of algebraic order two. Let us see what can be obtained with the three-stage scheme:

which is of algebraic order two. Its S and P functions are given by

$$(1+az)^{3}S(z) = 2 + [6a-1]z + [6a^{2}-2a+\frac{1}{2}(a_{2}+a_{3})+a_{2}c_{1}+a_{3}c_{2}]z^{2}$$

$$+[2a^{3}-a^{2}+a(\frac{1}{2}a_{2}+\frac{1}{2}a_{3}+a_{2}c_{1}+a_{3}c_{2})-a_{1}a_{3}(c_{1}+\frac{1}{2})]z^{3},$$

$$(1+az)^{3}P(z) = 1 + 3az + [3a^{2}+a_{2}c_{1}+a_{3}c_{2}-\frac{1}{2}(a_{2}+a_{3})]z^{2}$$

$$+[a^{3}-a_{1}a_{3}(c_{1}-\frac{1}{2})+a(a_{2}c_{1}+a_{3}c_{2}-\frac{1}{2}a_{2}-\frac{1}{2}a_{3})]z^{3}.$$

Identification of these functions with the pair $\{S_3^{(6,6)}(z), P_3^{(6,6)}(z) \equiv 1\}$ from Table 3.1 can be achieved by setting

$$c_1 = c_2 = \frac{1}{2}$$
, $a_1 = (a^2 - \frac{1}{6}a + \frac{1}{360})/a_3$, $a_2 = -a + \frac{1}{12} - a_3$

with a and a_3 free parameters.

The resulting scheme is sixth-order dispersive and, if $a > 0.656 \cdots$, it is *P*-stable. For the special *a*-values given in Table 3.1, its order of dispersion is raised to eight. In the numerical experiments we will choose $a_3 = \frac{1}{12} - a$ resulting in $a_2 = 0$.

Within the class of dissipative methods the parameters π_j^* in (3.2) can be employed for a further increase of the dispersion order. However, as the high-order dispersion relations are nonlinear expressions (see Table 2.1), we could no longer follow the analytical approach as was possible so far.

Therefore, starting with scheme (4.7) and imposing q = 10, we formulated the corresponding nonlinear system in terms of the parameters a, a_1 , a_2 , and a_3 . For a range of "realistic" c_1 and c_2 values these systems were solved numerically; among the large set of solutions, we selected the one with the largest (strong) stability interval. The resulting scheme is given by

which has strong stability interval (0, 19.30).

4.4. Reference method. In order to evaluate the merits of the methods of high dispersion order, we need a reference formula in which the parameters are utilized to obtain the highest possible algebraic order (with respect to the number of stages).

If we require a nonempty periodicity interval, then a suitable scheme is given by [15]

Both the algebraic and dispersion order are equal to four and the interval of periodicity is given by (0, 12). Note that this scheme is of comparable computational complexity as the methods of the previous sections, and hence a comparison is quite feasible.

5. Numerical experiments. To test the dispersive behaviour of the various schemes we implement the following test strategy. Let T_1 and T_{101} be the positions on the *t*-axis where the exact solution assumes its first and 101st zero, respectively; hence $T := T_{101} - T_1$ denotes the length of 50 oscillations of the true solution. This distance will be compared with its numerical analogue. However, in all experiments we use a fixed integration step h and, consequently, the "numerical zeros" will, in general, not coincide with a multiple of h. By using trigonometric interpolation based on neighbouring numerical values, the position of these "numerical zeros" can be simulated. In this way we calculate approximations to the positions of the first and 101st zero of the numerical solution, denoted by \tilde{T}_1 and \tilde{T}_{101} , respectively.

By means of this procedure, we annihilate the influence of the initial dispersion error (see the discussion in § 2.1). Moreover, possible dissipation errors are not taken into account. Hence, only the propagated dispersion error is measured.

In the tables of results we will give the values of T (if no analytical solution is available, this value is obtained by an integration with extremely small stepsize), the value of $\tilde{T} := \tilde{T}_{101} - \tilde{T}_1$, and (in parentheses) the number of correct digits in the relative error of \tilde{T} ; i.e.,

$$(5.1) cd := -\log_{10} |(T - \tilde{T})/T|.$$

Finally, the implicit relations occurring in the DIRKN methods are solved by Newton iteration with a sufficiently stringent stop criterion.

5.1. Linear problems with nonconstant frequency. As a first example we consider

(5.2)
$$\ddot{v}(t) + \ln(2+t)v(t) = 0, \quad t \ge 0, \quad v(0) = 0, \quad \dot{v}(0) = 1,$$

which can be considered as a model problem with slowly varying frequency $\omega \simeq [\ln{(2+t)}]^{1/2}$. For this problem the zeros of the exact solution are found to be $T_1 \simeq 2.83932438015$ and $T_{101} \simeq 157.2720560789$. In Table 5.1 we list the results of the various schemes for several values of h. From these results we conclude that the schemes of high dispersion order are much more efficient than the classical DIRKN method.

Our next example is in the same class of perturbed model equations; it is a widely-used test problem, provided by [6]

(5.3a)
$$\ddot{y}(t) + \left(100 + \frac{1}{4t^2}\right)y(t) = 0, \qquad t \ge 0.9$$

with the initial values taken from the "almost periodic" particular solution

(5.3b)
$$y(t) = t^{1/2} J_0(10t),$$

TABLE 5.1 \tilde{T} and (cd) values for problem (5.2); T = 154.43273169875.

Method	p q		h = 1	$h=\frac{1}{2}$	$h = \frac{1}{4}$	
(4.3)	2	6	154.734 (2.7)	154.4354 (4.8)	154.43275 (7.0)	
(4.5)	2	6	147.84 (1.4)	154.336 (3.2)	154.4322 (5.5)	
$(4.7), a = a^{(3)}$	2	8	154.4966 (3.4)	154.4329 (6.0)	154.432713 (6.9)	
(4.8)	2	10	154.593 (3.0)	154.4337 (5.2)	154.432747 (7.0)	
(4.9)	4	4	168.65 (1.0)	156.714 (1.8)	154.640 (2.9)	

 J_0 being the first-kind Bessel function. For the analytical zeros (beyond t = 0.9) we find $T_1 = 1.17915344391$ and $T_{101} = 32.59406213135$. The results for the various methods can be found in Table 5.2; they give rise to the same conclusions as in the previous example.

5.2. Nonlinear examples. To illustrate the behaviour of the schemes when applied to a nonmodel problem (that is, a problem which is not of the form (2.3)), we consider the nonlinear example

(5.4)
$$\ddot{y}(t) = -y^3(t), \quad t \ge 0, \quad y(0) = 0, \quad \dot{y}(0) = 1,$$

which has an oscillating solution with $T_1 = 3.11816949951$ and $T_{101} = 314.9351194459$. Table 5.3 contains the results for this problem. Here we observe that the methods which are *dissipative*, viz. (4.5) and (4.8), show a tremendous phase lag, despite their high dispersion order. This is explained if we consider the linearized right-hand side of (5.4), i.e., $-3y^2(t) \cdot y(t)$, and regard the term $-3y^2$, at least locally, as representing the term $-\omega^2$ in the model equation; then it is clear that a dissipative method will produce an oscillation with an increasing period. This explains the large values of \tilde{T} for these methods. The schemes with zero dissipation behave very accurately.

From this example we conclude that the methods profit from a high phase-lag order, even in nonmodel situations, but that zero dissipativity for such equations is of crucial importance.

As a second example of a nonmodel situation we consider the orbit equation [5]

(5.5a)
$$\ddot{y}_1(t) = -4t^2 y_1(t) - 2y_2(t) / \sqrt{y_1^2(t) + y_2^2(t)} , \qquad t \ge t_0 := \sqrt{\pi/2}.$$

Specifying the initial conditions $y_1(t_0) = 0$, $\dot{y}_1(t_0) = -\sqrt{2\pi}$, $y_2(t_0) = 1$, $\dot{y}_2(t_0) = 0$, we have the exact solution

(5.5b)
$$v_1(t) = \cos(t^2), \quad v_2(t) = \sin(t^2).$$

 $\begin{array}{c} {\rm TABLE~5.2} \\ \tilde{T}~and~(cd)~values~for~problem~(5.3);~T=31.41490868744. \end{array}$

Method	thod $p q h = \frac{1}{5}$		$h=\frac{1}{10}$	$h = \frac{1}{20}$	
(4.3)	2	6	31.4609 (2.8)	31.41536 (4.9)	31.4149145 (6.7)
(4.5)	2	6	30.245 (1.4)	31.3977 (3.3)	31.41476 (5.3)
$(4.7), a = a^{(3)}$	2	8	31.4234 (3.6)	31.414930 (6.2)	31.41490817 (7.8)
(4.8)	2	10	31.4290 (3.4)	31.414884 (6.1)	31.41490615 (7.1)
(4.9)	4	4	34.399 (1.0)	31.8746 (1.8)	31.4556 (2.9)

TABLE 5.3 \tilde{T} and (cd) values for problem (5.4); $T \approx 311.81694994639$.

Method	p q		$h=\frac{1}{2}$	$h=\frac{1}{4}$	$h = \frac{1}{8}$	
(4.3)	2	6	311.7961 (4.2)	311.81633 (5.7)	311.816910 (6.9)	
(4.5)	2	6	523.2 (0.2)	361.4 (0.8)	319.6 (1.6)	
$(4.7), a = a^{(3)}$	2	8	311.7956 (4.2)	311.81633 (5.7)	311.816910 (6.9)	
(4.8)	2	10	350.9 (0.9)	317.461 (1.7)	312.54 (2.6)	
(4.9)	4	4	313.60 (2.2)	311.971 (3.3)	311.8275 (4.5)	

We will test on the first component, $y_1(t)$, and its T-value is easily seen to be $T = \sqrt{203\pi/2} - \sqrt{3\pi/2}$. The results of the various methods are collected in Table 5.4. Here, an * means that the Newton process did not converge. Since the solution oscillates more rapidly as t increases, all methods have serious problems in accurately approximating T_{101} if they are applied with a large, constant stepsize, e.g., $h = \frac{1}{10}$. Consequently, the methods with high order of dispersion do not show any advantage over the standard method. However, as h decreases the order of dispersion becomes paramount to the algebraic order, even in this nonmodel situation, and the standard method is outperformed by the new methods.

The dispersion error introduced by the dissipation in the methods (4.5) and (4.8) is of less significance than it was in the previous example, but its influence in scheme (4.5) is noticeable. Note that the result obtained by the method (4.8) for $h = \frac{1}{40}$ is influenced by the error of the trigonometric interpolation.

5.3. A stiff example. In the examples shown so far, in all cases the stepsize was determined by accuracy considerations and there was no need for methods possessing a large stability/periodicity interval. As a matter of fact, we could equally well have chosen *explicit* RKN methods with high phase-lag order [9]. Now, we will test an example for which it is necessary to use an *implicit* method that is unconditionally stable or, preferably, *P*-stable. Hence, only the methods (4.4), (4.6), and $\{(4.7), a = \frac{2}{3}\}$ will be tested.

The equation describing the vibration in a cantilever bar is given by [19]

(5.6)
$$\frac{q}{\sigma} \frac{\partial^2 u}{\partial t^2} + EI \frac{\partial^4 u}{\partial x^4} = 0, \qquad 0 \le x \le l, \quad t \ge 0,$$

where q/g is the mass per unit length, E is the modulus of elasticity, and I denotes the moment of inertia. The solution of this equation can be taken to be of the form

(5.7)
$$u(t,x) = A_0 f(x) e^{i\omega t}, \qquad A_0 \in \mathbb{C}.$$

Substitution of (5.7) into (5.6) yields for f(x) an ordinary differential equation the general solution given by

(5.8)
$$f(x) = C_1 \cosh(\lambda x) + C_2 \sinh(\lambda x) + C_3 \cos(\lambda x) + C_4 \sin(\lambda x),$$

with $\lambda = (a\omega^2)^{1/4}$, a = q/gEI. The constants C_i are determined by boundary conditions of the form (see Fig. 1).

$$u = 0$$
, $u_x = 0$ at $x = 0$ and $u_{xx} = 0$, $u_{xxx} = 0$ at $x = l$.

Substitution of these conditions into (5.8) yields a homogeneous system for the constants C_i . To obtain a nontrivial solution the determinant must vanish, resulting in an equation for the frequency ω in (5.7)

(5.9)
$$\cosh (l(a\omega^2)^{1/4}) \cos (l(a\omega^2)^{1/4}) = -1,$$

Table 5.4 \tilde{T} and (cd) values for the first component of problem (5.5); T=15.686173985635.

Method	p q		$h = \frac{1}{10}$	$h = \frac{1}{20}$	$h = \frac{1}{40}$	
(4.3)	2	6	16.604 (1.2)	15.68766 (4.0)	15.686212 (5.6)	
(4.5)	2	6	*	15.5892 (2.3)	15.68396 (3.9)	
$(4.7), a = a^{(3)}$	2	8	16.280 (1.4)	15.68653 (4.6)	15.686197 (5.8)	
(4.8)	2	10	16.347 (1.4)	15.686131 (5.6)	15.6861527 (5.9)	
(4.9)	4	4	16.596 (1.2)	15.9738 (1.7)	15.7194 (2.7)	

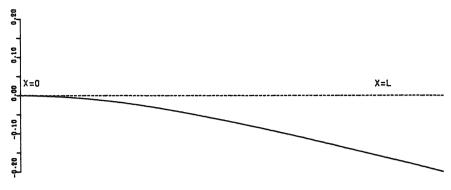


Fig. 1

which is approximately solved by

(5.10)
$$\omega^2 \frac{al^4}{\pi^4} = 0.126911803.$$

By choosing the appropriate initial conditions, i.e., u(0, x) = f(x) and $u_t(0, x) = 0$, we obtain the particular solution

$$(5.11) u(t, x) = f(x) \cdot \cos(\omega t),$$

where f(x) is given by

$$(5.12) \quad f(x) = A \left[\cosh(\lambda x) - \cos(\lambda x) - \frac{\cosh(\lambda l) + \cos(\lambda l)}{\sinh(\lambda l) + \sin(\lambda l)} \left(\sinh(\lambda x) - \sin(\lambda x) \right) \right],$$

with A a free parameter. In our test we choose the following data:

$$A = 0.1$$
, $l = 22$, $q/g = 50$, $EI = 10^4$,

resulting in $a = 5_{10^{-3}}$, $\omega \approx 0.10273546$, $T_1 \approx 15.2897$, $T_{101} \approx 3073.2335$.

Before we are able to apply our methods we first must semidiscretize (5.6). Therefore we define an equidistant grid $x_j := j\Delta$, $\Delta = l/N$, $(j = 1, \dots, N)$ and use the second-order approximation

$$\left. \frac{\partial^4 u}{\partial x^4} \right|_{x_i} \simeq \frac{1}{\Delta^4} (u_{j-2} - 4u_{j-1} + 6u_j - 4u_{j+1} + u_{j+2}).$$

Substituting the discretized boundary conditions, we arrive at

$$(5.13) \qquad \frac{d^{2}}{dt^{2}} \begin{bmatrix} u_{1} \\ u_{2} \\ u_{3} \\ \vdots \\ u_{N-2} \\ u_{N-1} \\ u_{N} \end{bmatrix} = -\frac{1}{a\Delta^{4}} \begin{bmatrix} 7 & -4 & 1 \\ -4 & 6 & -4 & 1 \\ 1 & -4 & 6 & -4 & 1 \\ & \ddots & \ddots & \ddots & \ddots \\ & & 1 & -4 & 6 & -4 & 1 \\ & & & 1 & -4 & 5 & -2 \\ & & & 2 & -4 & 2 \end{bmatrix} \begin{bmatrix} u_{1} \\ u_{2} \\ u_{3} \\ \vdots \\ u_{N-2} \\ u_{N-1} \\ u_{N} \end{bmatrix}$$

The eigenvalues of the Jacobian matrix in (5.13) are verified to be real. In our tests we used N = 20; for this value the spectral radius of the Jacobian is approximately 2160.

TABLE 5.5 \tilde{T} and (cd) values for the tenth component of (5.13); T = 3064.3996.

Method	р	q	h = 8	h = 4	h = 2	h = 1
(4.4)	2	4	3135.2 (1.6)	3070.7 (2.7)	3064.84 (3.8)	3064.424 (5.1)
(4.6)	2	4	3179.7 (1.4)	3076.3 (2.4)	3065.27 (3.6)	3064.460 (4.7)
$(4.7), a = \frac{2}{3}$	2	6	3095.3 (2.0)	3065.4 (3.5)	3064.43 (5.1)	3064.401 (6.3)

It should be observed that, due to the space discretization error, (5.11) is not exactly a solution to this ODE. Consequently, the values of T_1 and T_{101} corresponding to (5.13) differ slightly from the analytical values given above. A very accurate integration of this ODE (and testing on the 10th component) yielded $T_1 \approx 15.3289$ and $T_{101} \approx 3079.7285$. Table 5.5 shows the results obtained by the three DIRKN methods for several stepsizes.

6. Concluding remarks. In this paper we derived implicit Nyström methods with a friendly structure from the implementational/computational point of view, i.e., of diagonally implicit form. These methods share a relatively low algebraic order with a high phase-lag order; that is, they are aimed to integrate periodic initial value problems with small dispersion errors.

By a number of examples we have shown that problems possessing an oscillatory solution are more efficiently integrated by these new methods than by conventional methods with highest possible algebraic order. Although the theory is based on the linear, homogeneous model problem (2.3), this feature turned out to hold to a large extent in a nonmodel situation. However, in case of a nonlinear oscillator that largely deviates from the model problem in combination with a large stepsize, we may encounter the situation that the algebraic order is paramount to the order of dispersion; i.e., the total error is dominated by the usual truncation error rather than the dispersion error. In such cases the new methods do not show an advantage over standard methods. However, in the examples above, there is still a substantial gain in accuracy for the new methods.

Furthermore, we have seen that, especially for nonlinear problems (see § 5.2), methods with a nonempty periodicity interval usually yield more accurate results than the so-called dissipative methods.

Unless a large interval of periodicity is necessary, we recommend the second-order methods (4.3) and $\{(4.7), a = a^{(3)}\}$ having, respectively, order of dispersion six and eight. If large eigenvalues of the Jacobian are involved and *P*-stability is required, method $\{(4.7), a = \frac{2}{3}\}$ with q = 6 is probably the best choice.

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