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Diagonally Implicit Runge-Kutta-Nyström Methods for Oscillatory Problems

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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.

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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 deviced for the accurate integration of the initial value problem

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

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]. Firstly, we derive the dispersion relations in terms of the RKN parameters (see Section 2). Next, functions S and P characterizing the RKN method and satisfying the dispersion relations are constructed (Section 3). Finally, RKN methods which actually possess these highly dispersive functions S and P are computed (Section 4).

We present a number of second-order two- and three-stage methods with dispersion orders 4 up to 10. These methods are compared with a 'conventional' DIRKN method of order 4 using two stages, which requires a comparable computational effort. In Section 5, the methods are applied to a set of test problems, both linear and nonlinear examples. The new methods behave markedly more accurate than the conventional method (for example, a reduction of the phase-lag error by a factor 1000 is not an exception). It turned out that these large reduction factors are also obtained for the nonlinear problems, which considerably differ from the linear model problem on which the theory is based.

It should be remarked that recently a large number of papers has been published proposing methods with high order phase-lag. A few of them deal with first-order differential equations [1, 9, 12,] but the majority of the papers is 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 2, if P-stability (cf. Section 3.1) is required. To take this barrier, Cash [2], Thomas [18] and Chawla et al. [3, 4] considered hybrid variants of these LM methods, by introducing offstep points in the formulae to obtain methods which fit into the class of general multistep

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Runge-Kutta methods. Within this class it is possible to achieve high-order P-stable methods. In this connection, we also mention the papers of HAIRER [8] and of 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], which investigated multiderivative methods and the PC-type methods 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

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

have to be solved; obviously, this is unattractive from a computational point of view. One way to remove this deficiency, is to factor the matrix into a product of matrices. However, the coefficients in these matrices should be real, which in turn restricts the attainable order. For an extensive discussion on this subject, we refer to [2, 18].

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

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

$$\begin{aligned} Y_{nj} &= y_n + c_j h\dot{y}_n + h^2\sum_{l=1}^{m} a_{jl} f(t_n + c_l h, Y_{nl}), \qquad j = 1,\ldots,m, \\ y_{n+1} &= y_n + h\dot{y}_n + h^2\sum_{j=1}^{m} b_j f(t_n + c_j h, Y_{nj}), \\ \dot{y}_{n+1} &= \dot{y}_n + h\sum_{j=1}^{m} b'_j f(t_n + c_j h, Y_{nj}), \end{aligned} \tag{2.1}$$

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

By defining

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

the RKN method can be represented by the Butcher array

$$\begin{array}{c|c} \mathbf{c} & A \\ \hline & \mathbf{b}^T \\ & \mathbf{b}'^T \end{array} . \tag{2.1'}$$

2.1. Homogeneous test equation

In this subsection we consider the homogeneous test equation

$$\ddot{y} = -\omega^2 y, \quad \omega \in \mathbb{R}. \tag{2.3}$$

Application of (2.1) yields the recursion

$$\begin{aligned} y_{n+1} &= y_n + h\dot{y}_n - v^2 \mathbf{b}^T \mathbf{Y}_n, \\ h\dot{y}_{n+1} &= h\dot{y}_n - v^2 \mathbf{b}'^T \mathbf{Y}_n, \end{aligned} \tag{2.4a}$$

where

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

Elimination of the auxiliary vector $\mathbf{Y}_n$ yields

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

Following [9] we introduce the functions

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

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

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

and the *amplification error* or *dissipation* by

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

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 (cf. [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 which have a high order of dispersion. In addition, part 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

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

hence, the local truncation error $\tau(v)$ of this linear 2-steps method is defined by substitution of the exact solution of (2.3) into (2.5'):

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

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

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

We shall likewise call the RKN method dispersive and dissipative of order q and r, if, respectively

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

It should be remarked that (2.11) is a sufficient and necessary condition for a q-th order dispersive, r-th 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:*

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

(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, 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* $q \geq 2\lfloor (p+1)/2 \rfloor$ *and* $r \geq 2\lfloor (p+1)/2 \rfloor$.

(e) *If* $P(v^2) \equiv 1$ *then the orders of consistency and dispersion of S and P are equal.* □

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

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

In order to facilitate the construction of high-order dispersive functions S and P, we introduce the Taylor expansions of S and P:

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

and we express the order conditions (2.10) and (2.11) directly in terms of the coefficients σ_j and π_j. From the Tables 2.1 and 2.2 the dispersion and consistency relations are easily derived. It should be remarked that in the context of *explicit* RKN methods the dispersion relations were already derived in [9].

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

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

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

$$\sigma_j = \mathbf{b}^T A^{j-1}\mathbf{e} + \mathbf{b}'^T A^{j-1}\mathbf{c}. \tag{2.14}$$

The coefficients π_j are, in general, 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

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

so that

$$\pi_j = \mathbf{b}^T A^{j-1}\mathbf{e} + \mathbf{b}'^T A^{j-1}(\mathbf{c} - \mathbf{e}) = \sigma_j - \mathbf{b}'^T A^{j-1}\mathbf{e}. \tag{2.16}$$

It should be remarked that the simplifying condition $\mathbf{b}' = \beta\mathbf{b}$ or $\mathbf{c} = \gamma\mathbf{e}$, restricts the algebraic order of

the RKN method to 1 and 2 (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

In order to model forced oscillations the inhomogeneous test equation

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

is frequently used (cf. [7, 11, 17]). Application of the RKN method (2.1) yields the inhomogeneous recursion

$$\begin{bmatrix} y_{n+1} \\ h\dot{y}_{n+1} \end{bmatrix} = M(v^2) \begin{bmatrix} y_n \\ h\dot{y}_n \end{bmatrix} + ch^2 e^{i\omega_f t_n} \mathbf{g}, \tag{2.18}$$

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

$$\mathbf{g} := \begin{bmatrix} \mathbf{b}^T N^{-1} \mathbf{e}_f \\ \mathbf{b}'^T N^{-1} \mathbf{e}_f \end{bmatrix}, \qquad \mathbf{e}_f := (\exp(iv_f c_l)), \qquad v_f := h\omega_f . \tag{2.19}$$

It is easily verified that

$$\begin{bmatrix} y_n \\ h\dot{y}_n \end{bmatrix} = ch^2 e^{i\omega_f t_n} (e^{iv_f} I - M)^{-1} \mathbf{g} \tag{2.20}$$

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

$$\begin{bmatrix} y(t_n) \\ h\dot{y}(t_n) \end{bmatrix} = \frac{ch^2}{v^2 - v_f^2} e^{i\omega_f t_n} \begin{bmatrix} 1 \\ iv_f \end{bmatrix}. \tag{2.21}$$

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 $\alpha(v)$ which form the main source of inaccuracies when long interval integrations are performed.

3. Construction of Highly Dispersive 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 $a_{jj} = a$ for $j = 1,...,m$. For such methods, $S(z)$ assumes the form

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

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

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

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

The functions S and P of the special form (3.1) and (3.2), and being consistent and dispersive of

order p and q, will be denoted by $S_m^{(p,q)}$ and $P_m^{(p,q)}$.

3.1. Zero-dissipative methods

In this subsection 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. Such methods are said to have an *interval of periodicity* (cf. LAMBERT and WATSON [14]).

In Table 3.1 we have listed a few functions $S_m^{(p,q)}$ which were 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). (Notice that, by virtue of Theorem 2.1(e), $p = q$.)

We also listed the interval of periodicity defined by

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

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., $P(z) \equiv 1$

$m=1$: $S_1^{(2,2)}(z) = \dfrac{2+(2a-1)z}{1+az}$;

$a \geqslant 1/4$	$\Rightarrow q=2,\ H_0^2=\infty$
$a = 1/12$	$\Rightarrow q=4,\ H_0^2=6$

$m=2$: $S_2^{(4,4)}(z) = \dfrac{2+(4a-1)z+(2a^2-2a+1/12)z^2}{(1+az)^2}$;

$a > 1/4+\sqrt{6}/12$	$\Rightarrow q=4,\ H_0^2=\infty$
$a = 1/12+\sqrt{15}/60$	$\Rightarrow q=6,\ H_0^2\approx 6.43$
$a = 1/12-\sqrt{15}/60$	$\Rightarrow q=6,\ H_0^2\approx 21.85$

$m=3$: $S_3^{(6,6)}(z) = \dfrac{2+(6a-1)z+(6a^2-3a+1/12)z^2+(2a^3-3a^2+a/4-1/360)z^3}{(1+az)^3}$;

$a > .656...$	$\Rightarrow q=6,\ H_0^2=\infty$
$a = a^{(1)} = .2117520482855$	$\Rightarrow q=8,\ H_0^2\approx 6.64$
$a = a^{(2)} = .7657710662139_{10^{-2}}$	$\Rightarrow q=8,\ H_0^2\approx 9.33$
$a = a^{(3)} = .3059024105236_{10^{-1}}$	$\Rightarrow q=8,\ H_0^2\approx 24.15$

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 subsection. Consequently, there is no longer an interval of periodicity, but an *interval of strong stability* defined by

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

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 subsection. 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 2-stage zero-dissipative functions of Table 3.1.

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 $(0,\beta^2)$

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

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

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

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

$m=2$: $\quad S_2^{(3,q)}(z)=\dfrac{2+(4a-1)+(\pi_2^*+a^2-2a+1/12)z^2}{(1+az)^2}$,

$P_2^{(3,q)}(z)=\dfrac{1+2az+\pi_2^* z^2}{(1+az)^2}$; $q\geqslant 4$.

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

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

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

$a<\frac{1}{12}-\frac{1}{60}\sqrt{15} \Rightarrow \beta^2=12/(1-24a)$

For all other values of a we have $\beta^2=0$

(iii) $\left.\begin{array}{l}\pi_2^*=-a^2+a/3-1/180\\ \sigma_2(3\sigma_2-12a-4)-a(24a^2+3a-2)+31/105=0\\ \sigma_2=7/90+a/3-2a^2\end{array}\right\} \Rightarrow q=8$

$a=.3148024587598 \Rightarrow q=8,\ \beta^2=6.21$

$a=.0218432425854 \Rightarrow q=8,\ \beta^2=0$

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4. CONSTRUCTION OF HIGH-ORDER DISPERSIVE DIRKN METHODS

The construction of high-order dispersive DIRKN methods consists of the identification of the S and P functions of a given class of methods with one of the function pairs given in Section 3. In order to find a convenient expression for S and P the following lemma is helpful (cf. [12]):

LEMMA 4.1. *Let N be a nonsingular m by m matrix, and let $\mathbf{v}$ and $\mathbf{w}$ be m-dimensional vectors. Then*

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

By means of this lemma the inverse of the matrix $N=I+v^2A$ 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

$$\begin{array}{c|c} 1/2 & a \\ \hline & 1/2 \\ & 1 \end{array} . \tag{4.1}$$

The corresponding functions S and P are given by

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

For $a = 1/12$ 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 $a = 1/12$ 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 2:

$$\begin{array}{c|cc} c & a & \\ 1/2 & a_1 & a \\ \hline & 0 & 1/2 \\ & 0 & 1 \end{array} . \tag{4.2}$$

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 $c = 1/2$ and $a_1 = 1/12-a$, 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*

$$\begin{array}{c|cc} 1/2 & 1/12-\sqrt{15}/60 & \\ 1/2 & \sqrt{15}/60 & 1/12-\sqrt{15}/60 \\ \hline & 0 & 1/2 \\ & 0 & 1 \end{array} \tag{4.3}$$

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

$$\begin{array}{c|cc} 1/2 & 1/2 & \\ 1/2 & -5/12 & 1/2 \\ \hline & 0 & 1/2 \\ & 0 & 1 \end{array} . \tag{4.4}$$

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

$$\begin{array}{c|cc} \dfrac{24a^2+2a-13/30}{12a-1} & a & \\ 1/2 & 1/12-a & a \\ \hline & 0 & 1/2 \\ & 0 & 1 \end{array} . \tag{4.5}$$

Eighth-order dispersion is obtained for $a = .3148024587598$ 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*

$$\begin{array}{c|cc} \frac{12a^2+6a-1/2}{12a-1} & a & \\ 1/2 & 1/12-a & a \\ \hline & 0 & 1/2 \\ & 0 & 1 \end{array} \tag{4.6}$$

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

4.3. Two three-stage methods of algebraic order 2

Let us see what can be obtained with the three-stage scheme

$$\begin{array}{c|ccc} c_1 & a & & \\ c_2 & a_1 & a & \\ 1/2 & a_2 & a_3 & a \\ \hline & 0 & 0 & 1/2 \\ & 0 & 0 & 1 \end{array} \tag{4.7}$$

which is of algebraic order 2. Its S- and P-functions are given by

$$\begin{aligned} (1+az)^3 S(z) &= 2+[6a-1]z+[6a^2-2a+\tfrac{1}{2}(a_2+a_3)+a_2c_1+a_3c_2]z^2 \\ &\quad +[2a^3-a^2+a(\tfrac{1}{2}a_2+\tfrac{1}{2}a_3+a_2c_1+a_3c_2)-a_1a_3(c_1+\tfrac{1}{2})]z^3, \\ (1+az)^3 P(z) &= 1+3az+[3a^2+a_2c_1+a_3c_2-\tfrac{1}{2}(a_2+a_3)]z^2 \\ &\quad +[a^3-a_1a_3(c_1-\tfrac{1}{2})+a(a_2c_1+a_3c_2-\tfrac{1}{2}a_2-\tfrac{1}{2}a_3)]z^3. \end{aligned}$$

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

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

with a and a_3 free parameters.

The resulting scheme is sixth-order dispersive and, if $a > .656...$, 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 $a_3 = 1/12 - a$ 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 (cf. 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

$$\begin{array}{c|ccc} 1/2 & a & & \\ 3/10 & -.17329232352333 & a & \\ 1/2 & -.01271397498318 & .043727040749588 & a \\ \hline & 0 & 0 & 1/2 \\ & 0 & 0 & 1 \end{array} \tag{4.8}$$

$$a = .052320267566927$$

which has strong stability interval (0,19.30).

4.4. Reference method

In order to evaluate the merits of the highly dispersive methods 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]

$$\begin{array}{c|cc} \frac{1}{2}+\frac{1}{6}\sqrt{3} & \frac{1}{6}+\frac{1}{12}\sqrt{3} & \\ \frac{1}{2}-\frac{1}{6}\sqrt{3} & -\frac{1}{6}\sqrt{3} & \frac{1}{6}+\frac{1}{12}\sqrt{3} \\ \hline & \frac{1}{4}-\frac{1}{12}\sqrt{3} & \frac{1}{4}+\frac{1}{12}\sqrt{3} \\ & \frac{1}{2} & \frac{1}{2} \end{array} . \tag{4.9}$$

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

In order to test the dispersive behaviour of the various schemes we implemented 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 is to be compared with its numerical analogue. However, in all experiments we used 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 calculated 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 (cf. the discussion in Section 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.

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

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

5.1. Linear problems with non-constant frequency

As a first example we consider

$$\ddot{y}(t)+\ln(2+t)y(t) = 0,\ t\geqslant 0,\ y(0) = 0,\ \dot{y}(0) = 1, \tag{5.2}$$

which can be considered as a model problem with slowly varying frequency $\omega \simeq [\ln(2+t)]^{\frac{1}{2}}$. 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.

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)
(5.1)	4	4	168.65 (1.0)	156.714 (1.8)	154.640 (2.9)

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

$$\ddot{y}(t)+(100+\frac{1}{4t^2})y(t) = 0,\ t \geqslant 0.9 \tag{5.3a}$$

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

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

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.

TABLE 5.2. $\tilde{T}$ and (cd) values for problem (5.3); $T = 31.41490868744$

method	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)
(5.1)	4	4	34.399 (1.0)	31.8746 (1.8)	31.4556 (2.9)

5.2. Nonlinear examples

To illustrate the behaviour of the schemes when applied to a nonmodel problem, we consider the nonlinear example

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

which has an oscillating solution with $T_1 \simeq 3.11816949951$ and $T_{101} \simeq 314.9351194459$. Table 5.3 contains the results for this problem. Here we observe that the methods which

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

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)
(5.1)	4	4	313.60	(2.2)	311.971	(3.3)	311.8275	(4.5)

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 equation (5.4), i.e. $-3y^2(t)\cdot y(t)$ and regard the term $-3y^2$, at least locally, as to represent 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.

We conclude from this example 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]

$$\begin{aligned} \ddot{y}_1(t) &= -4t^2 y_1(t) - 2y_2(t)/\sqrt{y_1^2(t)+y_2^2(t)} \\ \ddot{y}_2(t) &= -4t^2 y_2(t) + 2y_1(t)/\sqrt{y_1^2(t)+y_2^2(t)} \end{aligned},\quad t \geqslant t_0 := \sqrt{\pi/2}. \tag{5.5a}$$

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

$$y_1(t) = \cos(t^2),\ y_2(t) = \sin(t^2). \tag{5.5b}$$

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

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)
(5.1)	4	4	16.596 (1.2)	15.9738 (1.7)	15.7194 (2.7)

a large, *constant* stepsize, e.g. $h=1/10$. 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. It should be remarked that the result obtained by the method (4.8) for $h=1/40$ is influenced by the error of the trigonometric interpolation.

5.3. A stiff example

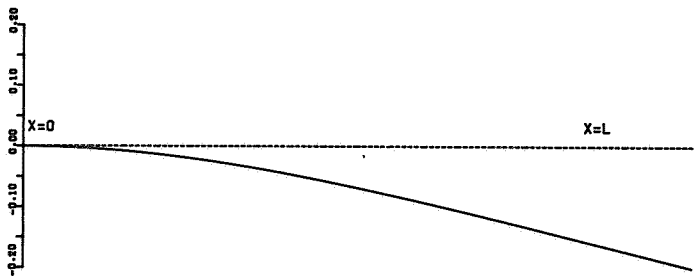
In the examples shown sofar, the stepsize was in all cases determined by accuracy considerations and there was no need for methods possessing a large stability/periodicity interval. As a matter of fact, we could equally well have chosen *explicit* RKN methods with high phase-lag order [9]. Now, we will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

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

$$\frac{q}{g}\frac{\partial^2 u}{\partial t^2} + EI\frac{\partial^4 u}{\partial x^4} = 0, \quad 0 \leqslant x \leqslant l, \ t \geqslant 0, \tag{5.6}$$

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 of the form

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



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

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

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

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

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 which results in an equation for the frequency ω in (5.7)

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

which is approximately solved by

$$\omega^2\frac{al^4}{\pi^4} = .126911803. \tag{5.10}$$

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

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

where $f(x)$ is given by

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

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 $a = 5_{10^{-3}}$, $\omega\simeq.10273546$, $T_1\simeq 15.2897$, $T_{101}\simeq 3073.2335$.

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

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

Substituting the discretized boundary conditions, we arrive at

$$\frac{d^2}{dt^2}\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \cdot \\ \cdot \\ \cdot \\ u_{N-2} \\ u_{N-1} \\ u_N \end{bmatrix} = -\frac{1}{a\Delta^4}\begin{bmatrix} 7 & -4 & 1 & & & & & & \\ -4 & 6 & -4 & 1 & & & & & \\ 1 & -4 & 6 & -4 & 1 & & & & \\ & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & \\ & & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \\ & & & 1 & -4 & 6 & -4 & 1 & \\ & & & & 1 & -4 & 5 & -2 & \\ & & & & & 2 & -4 & 2 & \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \cdot \\ \cdot \\ \cdot \\ u_{N-2} \\ u_{N-1} \\ u_N \end{bmatrix}. \tag{5.13}$$

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.

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) slightly differ from the analytical values given above. A very accurate integration of this ODE (and testing on the 10th

component) yielded $T_1 \simeq 15.3289$ and $T_{101} \simeq 3079.7285$. Table 5.5 shows the results obtained by the three DIRKN methods for several stepsizes.

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

method	p	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),$a=2/3$	2	6	3095.3 (2.0)	3065.4 (3.5)	3064.43 (5.1)	3064.401 (6.3)

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. This feature turned out to hold even in nonmodel situation.

Furthermore, we have seen that, especially for nonlinear problems, (cf. Section 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 $\{(4.7), a = a^{(3)}\}$ which have respectively order of dispersion 6 and 8. If large eigenvalues of the Jacobian are involved and P-stability is a requisite, method $\{(4.7), a = 2/3\}$ with $q = 6$ is probably the best choice.

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