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Department of Numerical Mathematics Report NM-R8504 April

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# Explicit Runge-Kutta (-Nyström) Methods with Reduced Phase Errors for Computing Oscillating Solutions

P.J. van der Houwen, B.P. Sommeijer

We construct explicit Runge-Kutta (-Nyström) methods for the integration of first (and second) order differential equations having an oscillatory solution. Special attention is paid to the *phase errors* (or *dispersion)* of the dominant components in the numerical oscillations when these methods are applied to a linear, homogeneous test model. RK(N) methods are constructed which are dispersive of orders up to 10, whereas the (algebraic) order of accuracy is only 2 or 3. Application of these methods to semi-discretized hyperbolic equations and to equations describing free and weakly forced oscillations, reveals that the phase errors can significantly be reduced.

*1980 Mathematics subject classification: 65L05.*
*1982 CR Categories: G.1.7, G.1.8*
*Key words & Phrases:* numerical analysis, ordinary differential equations, periodic solutions, Runge-Kutta methods.

## 1. Introduction

We shall discuss the construction of special Runge-Kutta (-Nyström) methods for integrating systems of ODEs of the form

$$\frac{d^k y}{dt^k} = f(t,y),\ k = 1,2. \tag{1.1}$$

The methods are designed in such a way that for *linear* systems with $f(t,y) = Ay$, where $A$ is skew symmetric if $k = 1$ and symmetric if $k = 2$, the phase error of the low frequencies in the numerical solution is small. Methods possessing this property are suitable for long interval integration of, for example, semi-discrete hyperbolic equations with smooth solutions. With this application in mind, and in view of the very large systems that arise when hyperbolic equations are semi-discretized, we will concentrate on *explicit* methods in order to reduce storage requirements; the disadvantage of a restricted maximal integration step is partly compensated by the arrival of vector computers on which explicit methods can be implemented with great efficiency.

In this paper we will use the test equation

$$\frac{d^k y}{dt^k} = (i\omega)^k y,\quad \omega \text{ real.} \tag{1.2}$$

By comparing the exact and numerical solution for this equation, and by requiring that these solutions are in phase with maximal possible order in the step size $h$, we derive the so-called *dispersion relations,* from which the Runge-Kutta (-Nyström) methods can be constructed. These methods will be illustrated by applying them to semi-discretized hyperbolic equations and to equations describing free or weakly forced oscillations.

The reduction of phase errors has been studied in, e.g., [1], [8], [9] and [10]. In [1] Brusa and Nigro construct an implicit one-step method that is third order accurate and that computes with small phase errors the solutions of the (inhomogeneous) test equation

Report NM-R8504
Centre for Mathematics and Computer Science
P.O. Box 4079, 1009 AB Amsterdam, The Netherlands

$$\frac{d^k y}{dt^k} = (i\omega)^k y + ve^{i\omega_p t}. \tag{1.3}$$

In [10] Thomas uses this test equation (with $k = 2$) for extending the families of multistep Runge-Kutta methods of Cash [2] and of Chawla [3] such that the particular solution

$$y_p(t) := \frac{v}{\omega^2 - \omega_p^2} \exp(i\omega_p t) \tag{1.4}$$

is integrated with a phase error of high order as $h \to 0$. Finally, in [8] and [9] Strehmel and Weiner derive for Runge-Kutta-Nyström and Rosenbrock type methods a (dispersion) relation such that the particular solution $y_p(t)$ is computed with zero phase error for given $\omega$ and $\omega_p$.

The extension of our analysis of Runge-Kutta(-Nyström) methods to the inhomogeneous test equation (1.3) will be the subject of a future paper.

A few preliminary results of the analysis presented in this paper have already been reported at the "4° Tagung Numerische Behandlung von gewöhnlichen Differentialgleichungen" organized by Prof.Dr.sc. R. März of the Humboldt-University-Berlin.

## 2. Dispersion and dissipation in Runge-Kutta(-Nystrom) methods

### *2.1 The order of dispersion and dissipation*

For first-order equations ($k = 1$ in (1.1)) we write the $m$-stage, explicit Runge-Kutta method in the form

$$\begin{aligned} y_n^{(0)} &= y_{n-1} \\ y_n^{(j)} &= y_{n-1} + h\sum_{l=0}^{j-1} \lambda_{j,l} f(t_{n-1} + \mu_l h, y_n^{(l)}), \quad j = 1,\ldots,m, \\ y_n &:= y_n^{(m)}. \end{aligned} \tag{2.1}$$

Here, $\mu_0 = 0$ and $y_n, y_{n-1}$ denote approximations to $y(t_n)$ and $y(t_n - h)$, respectively. Application of (2.1) to (1.2) with $k = 1$ yields the numerical solution

$$y_n = \tilde{a}^n y_0, \quad \tilde{a} := A_m(v^2) + ivB_m(v^2), \quad v := \omega h, \tag{2.2}$$

where $A_m$ and $B_m$ are polynomials in $v^2$, completely defined by the Runge-Kutta parameters $\lambda_{j,l}$; $\tilde{a} = \tilde{a}(v)$ will be called the *amplification factor.* A comparison of (2.2) with the solution of (1.2), i.e. $y(t_n) = y_0 \exp(inv)$, leads us to the following definition:

Definition 2.1. In the Runge-Kutta method (2.1) the quantities

$$\phi(v) := v - \arg[\tilde{a}(v)], \quad \alpha(v) := 1 - |\tilde{a}(v)|$$

are respectively called the *dispersion* (or *phase error* or *phase lag)* and the *amplification error.* If $\phi(v) = 0(v^{q+1})$ and $\alpha(v) = 0(v^{r+1})$ then the method is said to be *dispersive of order* $q$ and *dissipative of order* $r$. □

It follows from (2.2) that

$$\phi(v) = v - \arctan\left(v\frac{B_m(v^2)}{A_m(v^2)}\right), \quad \alpha(v) = 1 - \sqrt{A_m^2(v^2) + v^2 B_m^2(v^2)}. \tag{2.3}$$

Next we consider the $m$-stage, explicit Runge-Kutta-Nyström method for (1.1) with $k = 2$; we write this method in the form

$$\begin{aligned} y_n^{(0)} &= y_{n-1}, \\ y_n^{(j)} &= y_{n-1} + \mu_j h\dot{y}_{n-1} + h^2\sum_{l=0}^{j-1} \lambda_{j,l} f(t_{n-1} + \mu_l h, y_n^{(l)}), \quad j = 1,\ldots,m, \end{aligned}$$

$$y_n := y_n^{(m)}, \quad \dot{y}_n := \dot{y}_{n-1} + h\sum_{l=0}^{m-1} \lambda_l' f(t_{n-1} + \mu_l h, y_n^{(l)}), \tag{2.4}$$

where $\mu_0 = 0$ and $\mu_m = 1$. For the test equation (1.2) with $k = 2$ we obtain the numerical solution

$$\begin{bmatrix} y_n \\ h\dot{y}_n \end{bmatrix} = M^n \begin{bmatrix} y_0 \\ h\dot{y}_0 \end{bmatrix}, \quad M := \begin{bmatrix} A_m(v^2) & B_m(v^2) \\ A_m^*(v^2) & B_m^*(v^2) \end{bmatrix}, \quad v := \omega h, \tag{2.5}$$

where $A_m$, $A_m^*$, $B_m$ and $B_m^*$ are again polynomials in $v^2$, determined by the parameters in (2.4). The eigenvalues of $M$ will be called the *amplification factors* of the Runge-Kutta-Nyström method and are denoted by $\tilde{a}_+$ and $\tilde{a}_-$; the corresponding eigenvectors are given by

$$\mathbf{e}_\pm = (1, e_\pm)^T, \quad e_\pm := \frac{A_m^*(v^2)}{\tilde{a}_\pm - B_m^*(v^2)}.$$

In terms of $\tilde{a}_\pm$ and $e_\pm$ the numerical solution $y_n$ is given by

$$y_n = \tilde{c}_+(\tilde{a}_+)^n + \tilde{c}_-(\tilde{a}_-)^n, \quad \tilde{c}_+ := -\frac{e_- y_0 - h\dot{y}_0}{e_+ - e_-}, \quad \tilde{c}_- := \frac{e_+ y_0 - h\dot{y}_0}{e_+ - e_-} \tag{2.5'}$$

We compare this discrete solution with the continuous solution

$$y(t_n) = c_+(e^{iv})^n + c_-(e^{-iv})^n, \quad c_\pm := \tfrac{1}{2} y_0 \pm \frac{-i}{2\omega}\dot{y}_0. \tag{2.6}$$

Assuming that the amplification factors $\tilde{a}_\pm$ are complex conjugate we may write

$$\tilde{c}_\pm = |\tilde{c}|e^{\pm i\tilde{\psi}}, \quad \tilde{a}_\pm = |\tilde{a}|e^{\pm i\tilde{v}}$$

and similarly

$$c_\pm = |c|e^{\pm i\psi}, \quad a_\pm = e^{\pm iv}.$$

On substitution into (2.5') and (2.6) we find

$$y_n = 2|\tilde{c}||\tilde{a}|^n \cos(\tilde{\psi} + n\tilde{v}), \tag{2.5''}$$

$$y(t_n) = 2|c|\cos(\psi + nv). \tag{2.6'}$$

These expressions lead us to the following definition:

DEFINITION 2.2. In the Runge-Kutta-Nyström method (2.4) the quantities

$$\phi_0 := \psi - \tilde{\psi}, \quad \phi(v) := v - \tilde{v}, \quad \alpha_0 := |c| - |\tilde{c}|, \quad \alpha(v) := 1 - |\tilde{a}|$$

are respectively called: *initial dispersion, (propagated) dispersion, initial amplification error* and *(propagated) amplification error.* □

The initial dispersion and the initial amplification error are introduced by the differences $c_\pm - \tilde{c}_\pm$ determined by the initial values $y_0$ and $\dot{y}_0$. If these differences are $0(v^s)$ then the initial dispersion and initial amplification error are both $0(v^s)$ as $v \to 0$. These errors are not propagated in the numerical computations. In the following, $p$, $q$, $r$, $s$ denote the orders of accuracy, of dispersion, of amplification error, and of initial dispersion, respectively.

The errors $\phi(v)$ and $\alpha(v)$ accumulate in the numerical process and are therefore a cause of inaccuracies if many integration steps are performed. (This assertion also applies to the errors $\phi(v)$ and $\alpha(v)$ defined in Definition 2.1.) It follows from (2.5) that

$$\phi(v) = v - \arccos\left[\frac{S(v^2)}{2\sqrt{P(v^2)}}\right], \quad \alpha(v) = 1 - \sqrt{P(v^2)}, \tag{2.7}$$

where

$$S(\nu^2) := A_m(\nu^2) + B_m^*(\nu^2),$$
$$P(\nu^2) := A_m(\nu^2)B_m^*(\nu^2) - A_m^*(\nu^2)B_m(\nu^2).$$

In this paper we will concentrate on increasing the order of dispersion $q$ (defined by $\phi(\nu) = 0(\nu^{q+1})$). In the case of second-order equations we will maximize $q$ under the additional requirement of zero dissipation (i.e. $P(\nu^2) \equiv 1$ in (2.7)).

*2.2 Runge-Kutta methods*

In the following we will write

$$A_m(z) = 1 - \beta_2 z + \beta_4 z^2 \ldots$$
$$B_m(z) = 1 - \beta_3 z + \beta_5 z^2 \ldots, \tag{2.8}$$

where $\beta_j = 0$ for $j > m$. We want to express the conditions for dispersion of order $q$ in terms of the parameters $\beta_j$, $j = 2,\ldots,m$.

THEOREM 2.1. The Runge-Kutta method is dispersive of order $q = 2q_0$ if the parameters $\beta_j$, $j = 2,\ldots,m$, satisfy the relations

$$\gamma_{2j} - \gamma_{2j-2}\beta_2 + \gamma_{2j-4}\beta_4 - \ldots + (-1)^j \gamma_0 \beta_{2j} + (-1)^{j+1}\beta_{2j+1} = 0 \tag{2.9}$$

for $j = 1,\ldots,q_0 - 1$; here the coefficients $\gamma_{2l}$ are defined by the Taylor expansion

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

and

$$\beta_j = 0 \text{ for } j > m.$$

PROOF. From the definition of $\phi(\nu)$ it follows that, if

$$\nu \frac{B_m(\nu^2)}{A_m(\nu^2)} = \tan(\nu) - c\nu^{q+1}, \; c \text{ bounded as } \nu \to 0,$$

then

$$\phi(\nu) = \nu - \arctan[\tan(\nu) - c\nu^{q+1}] = c\nu^{q+1} + 0(\nu^{q+3}),$$

so that the method is dispersive of order $q$. Substitution of (2.8) and expanding $\tan(\nu)$ in a Taylor series leads to (2.9). □

COROLLARY 2.1. The maximal attainable order of dispersion of an $m$-stage, $p$-th order, explicit Runge-Kutta method is $q = 2(m - p + \lfloor (p+1)/2 \rfloor)$; here, $\lfloor x \rfloor$ denotes the integer part of $x$.

PROOF. From (2.2) and (2.8) it follows that a $p$-th order method necessarily satisfies the order conditions

$$\beta_j = \frac{1}{j!}, \quad j = 2,\ldots,p. \tag{2.10}$$

Hence, an $m$-stage, $p$-th order method has $m - p$ free parameters $\beta_j$. If these parameters satisfy (2.9), the order of dispersion is increased by $2(m-p)$. It can be shown that any $p$-th order method has already an order of dispersion $2\lfloor (p+1)/2 \rfloor$, whatever the parameters $\beta_{p+1}, \cdots, \beta_m$ are. Thus, the total order of dispersion can be increased to $2\lfloor (p+1)/2 \rfloor + 2(m-p)$. This completes the proof of Corollary 2.1. □

In Table 2.1a the dispersion relations (2.9) are listed for a few values of $p$ and $q$; in Table 2.1b the corresponding error constants are given.

TABLE 2.1a. Dispersion relations in terms of the parameters $\beta_j$

| Order | $q \geqslant$ | |
|---|---|---|
| $p = 1$ | 4 | $\beta_2 - \beta_3 = 1/3$ |
| | 6 | $\beta_2 - 3\beta_4 + 3\beta_5 = 2/5$ |
| | 8 | $2\beta_2 - 5\beta_4 + 15\beta_6 - 15\beta_7 = 17/21$ |
| | 10 | $17\beta_2 - 42\beta_4 + 105\beta_6 - 315\beta_8 + 315\beta_9 = 62/9$ |
| | 12 | $62\beta_2 - 153\beta_4 + 378\beta_6 - 945\beta_8 + 2835(\beta_{10} - \beta_{11}) = \frac{1382}{55}$ |
| $p = 2,3$ | 4 | $\beta_2 = 1/2,\ \beta_3 = 1/6$ |
| | 6 | $\beta_4 - \beta_5 = 1/30$ |
| | 8 | $\beta_4 - 3\beta_6 + 3\beta_7 = 4/105$ |
| | 10 | $2\beta_4 - 5\beta_6 + 15\beta_8 - 15\beta_9 = 29/378$ |
| | 12 | $17\beta_4 - 42\beta_6 + 105\beta_8 - 315\beta_{10} + 315\beta_{11} = 323/495$ |
| $p = 4,5$ | 6 | $\beta_2 = 1/2,\ \beta_3 = 1/6,\ \beta_4 = 1/24,\ \beta_5 = 1/120$ |
| | 8 | $\beta_6 - \beta_7 = 1/840$ |
| | 10 | $\beta_6 - 3\beta_8 + 3\beta_9 = 1/756$ |
| | 12 | $6\beta_6 - 15\beta_8 + 45\beta_{10} - 45\beta_{11} = 221/27720$ |

TABLE 2.1.b. Error constants $c$ in the dispersion $\phi(\nu) = c\nu^{q+1} + 0(\nu^{q+3})$

| $q$ | $c$ |
|---|---|
| 4 | $-\beta_5 + \beta_4 - \frac{1}{3}\beta_2 + 2/15$ |
| 6 | $\beta_7 - \beta_6 + \frac{1}{3}\beta_4 - 2\beta_2/15 + 17/315$ |
| 8 | $-\beta_9 + \beta_8 - \frac{1}{3}\beta_6 + 2\beta_4/15 - 17\beta_2/315 + \gamma_8$ |
| 10 | $\beta_{11} - \beta_{10} + \frac{1}{3}\beta_8 - 2\beta_6/15 + 17\beta_4/315 - \gamma_8\beta_2 + \gamma_{10}$ |
| 12 | $-\beta_{13} + \beta_{12} - \frac{1}{3}\beta_{10} + 2\beta_8/15 - 17\beta_6/315 + \gamma_8\beta_4 - \gamma_{10}\beta_2 + \gamma_{12}$ |

*2.3 Runge-Kutta-Nyström methods with zero dissipation*

We shall say that a Runge-Kutta-Nyström method has *zero dissipation* at a point $\nu$ if $\alpha(\nu) = 0$ where $\alpha(\nu)$ is defined in Definition 2.2; thus, the numerical solution of our test equation, specified in (2.5″), assumes the form $y_n = 2|\tilde{c}|\cos(\tilde{\psi} + n\nu)$. This means that, except for some initial amplification due to $|\tilde{c}|$, there is no dissipation (negative or positive) during the numerical calculation of the solution of equation {(1.2), $k = 2$}. The interval $0 \leqslant \nu^2 \leqslant \beta^2$ where $|\tilde{a}| = |\tilde{a}(\nu)| = 1$ and $\tilde{a}_+(\nu) \neq \tilde{a}_-(\nu)$, is called the *interval of periodicity* or the *interval of zero dissipation.*

A necessary condition for a non-empty interval of periodicity is $P(z) \equiv 1$, (cf. (2.7)). In this section we consider methods with $P(z) \equiv 1$, thereby simplifying the analysis considerably.

Let us write the polynomial $S(z)$, introduced in (2.7), in the form

$$S(z) = 2 - \sigma_1 z + \sigma_2 z^2 - \ldots,\ \sigma_j = 0 \text{ for } j > m. \tag{2.11}$$

The analogue of Theorem 2.1 becomes:

THEOREM 2.2. Let the Runge-Kutta-Nyström method be such that

$$P(z) := A_m(z)B_m^*(z) - A_m^*(z)B_m(z) \equiv 1. \tag{2.12}$$

Then the method in dispersive of order $q = 2q_0$ if the parameters $\sigma_j$ are given by

$$\sigma_j = \frac{2}{(2j)!},\ j = 1,\ldots,q_0. \tag{2.13}$$

PROOF. From (2.11) and (2.13) it follows that

$$S(\nu^2) = 2\cos(\nu) + 0(\nu^{2q_0+2}).$$

Hence,

$$\phi_\pm(\nu) = \pm[\nu - \arccos(\frac{2\cos(\nu) + 0(\nu^{2q_0+2})}{2\sqrt{P(\nu^2)}})]$$

$$= \pm[\nu - \arccos(\cos(\nu) + 0(\nu^{q+2}))] = 0(\nu^{q+1}). \quad \square$$

Since $S(z)$ is at most of degree m, it follows from Theorem 2.2 that the maximal attainable order of dispersion is $q = 2m$. We observe that the consistency conditions will not conflict with the dispersion relations (2.13). In fact, part of the consistency conditions coincide with the dispersion relations (cf.(2.9)).

*2.4 Dissipative Runge-Kutta-Nyström methods*

By dropping the condition of perodicity intervals, the order of dispersion can be increased. Writing

$$P(z) = 1 - \pi_1 z + \pi_2 z^2 - \pi_3 z^3 + \ldots,\ \pi_j = 0 \text{ for } j > m \tag{2.14}$$

and proceeding as in Section 2.2, we arrive at the dispersion relations

TABLE 2.2a. Dispersion relations in terms of the parameters $\sigma_j$ and $\pi_j$

| Order | $q \geqslant$ | |
|---|---|---|
| $p = 1$ | 2 | $\sigma_1 - \pi_1 = 1$ |
| | 4 | $\sigma_1^2 + 4\sigma_2 - 4\pi_1 - 4\pi_2 = 4/3$ |
| | 6 | $6\sigma_1\sigma_2 + 12\sigma_3 - 4\pi_1 - 12\pi_2 - 12\pi_3 = 8/15$ |
| | 8 | $45\sigma_2^2 + 90\sigma_1\sigma_3 + 180\sigma_4 - 8\pi_1 - 60\pi_2 - 180\pi_3 - 180\pi_4 = 4/7$ |
| | 10 | $45\sigma_2\sigma_3 + 45\sigma_1\sigma_4 + 90\sigma_5 - 2\pi_1/7 - 4\pi_2 - 30\pi_3 - 90\pi_4 - 90\pi_5 = 4/315$ |
| | 12 | $315\sigma_3^2 + 1260\sigma_6 + 630\sigma_1\sigma_5 + 630\sigma_2\sigma_4 - 8\pi_1/45 - 4\pi_2 - 56\pi_3$ $-420\pi_4 - 1260\pi_5 - 1260\pi_6 = 8/1485$ |
| $p = 2,3$ | 2 | $\sigma_1 = 1,\ \pi_1 = 0$ |
| | 4 | $\sigma_2 - \pi_2 = 1/12$ |
| | 6 | $\sigma_2 + 2\sigma_3 - 2\pi_2 - 2\pi_3 = 4/45$ |
| | 8 | $3\sigma_2^2 + 6\sigma_3 + 12\sigma_4 - 4\pi_2 - 12\pi_3 - 12\pi_4 = 4/105$ |
| | 10 | $45\sigma_2\sigma_3 + 45\sigma_4 + 90\sigma_5 - 4\pi_2 - 30\pi_3 - 90\pi_4 - 90\pi_5 = 4/315$ |
| | 12 | $315\sigma_3^2 + 1260\sigma_6 + 630\sigma_5 + 630\sigma_2\sigma_4 - 4\pi_2 - 56\pi_3 - 420\pi_4$ $-1260\pi_5 - 1260\pi_6 = 8/1485$ |
| $p = 4,5$ | 4 | $\sigma_1 = 1,\ \sigma_2 = 1/12,\ \pi_1 = \pi_2 = 0$ |
| | 6 | $\sigma_3 - \pi_3 = 1/360$ |
| | 8 | $\sigma_3 + 2\sigma_4 - 2\pi_3 - 2\pi_4 = 29/10080$ |
| | 10 | $5\sigma_3 + 60\sigma_4 + 120\sigma_5 - 40\pi_3 - 120\pi_4 - 120\pi_5 = 16/945$ |
| | 12 | $630\sigma_3^2 + 2520\sigma_6 + 1260\sigma_5 + 105\sigma_4 - 112\pi_3 - 840\pi_4$ $-2520\pi_5 - 2520\pi_6 = 16/1485$ |

listed in Table 2.2a. We observe that in a $p$-th order method the amplification factors $\tilde{a}_\pm$ satisfy the relation

$$\tilde{a}_\pm = \exp(\pm i\nu) + 0(\nu^{p+1})$$

so that

$$S(\nu^2) = 2\cos(\nu) + 0(\nu^{p+1}),\quad P(\nu^2) = 1+0(\nu^{p+1});$$

this has been used in the dispersion relations of Table 2.2a. In Table 2.2b we have listed the corresponding error constants.

TABLE 2.2b. Error constants $c$ in the dispersion $\phi(\nu) = c\nu^{q+1} + 0(\nu^{q+3})$

| $q$ | $c$ |
|---|---|
| 2 | $[\sigma_1^2+4\sigma_2-4\pi_1-4\pi_2-4/3]/8$ |
| 4 | $-[6\sigma_1\sigma_2+12\sigma_3-4\pi_1-12\pi_2-12\pi_3-8/15]/24$ |
| 6 | $[45\sigma_2^2+90\sigma_1\sigma_3+180\sigma_4-8\pi_1-60\pi_2-180\pi_3-180\pi_4-4/7]/360$ |
| 8 | $-[45\sigma_2\sigma_3+45\sigma_1\sigma_4+90\sigma_5-2\pi_1/7-4\pi_2-30\pi_3-90\pi_4-90\pi_5-4/315]/180$ |
| 10 | $[315\sigma_3^2+1260\sigma_6+630\sigma_1\sigma_5+630\sigma_2\sigma_4-8\pi_1/45-4\pi_2-56\pi_3$ $-420\pi_4-1260\pi_5-1260\pi_6-8/1485]/2520$ |

*2.5 Reduction of phase errors of known frequencies*

Suppose that it is known in advance that Fourier components $\exp(i\omega t)$ with $\omega\in[\underline{\omega},\bar{\omega}]$ are dominating in the exact solution. Then, it follows from Definition 2.1 that we can reduce the corresponding phase errors in the numerical solution by minimizing the dispersion function $\phi(\nu)$ on the interval $[\underline{\nu},\bar{\nu}]$: $= h[\underline{\omega},\bar{\omega}]$. If $\phi(\nu)$ would be a *polynomial,* then this minimax problem is solved by identifying $\phi(\nu)/\nu$ with a Chebyshev polynomial in $\nu^2$, shifted to the interval $[\underline{\nu},\bar{\nu}]$ (notice that $\phi(\nu)/\nu$ is an *even* function). Such an identification is accomplished by assigning to $\phi(\nu)$ the same zeros as this shifted Chebyshev polynomial possesses, i.e. the zeros

$$z_j := [\tfrac{1}{2}\bar{\nu}^2 + \tfrac{1}{2}\underline{\nu}^2 + \tfrac{1}{2}(\bar{\nu}^2-\underline{\nu}^2)\cos(\frac{2j-1}{2q_0}\pi)]^{\frac{1}{2}},\quad j = 1,...,q_0\,, \tag{2.15}$$

where $q_0$ is the number of free parameters in $\phi(\nu)$. We now assume that the location of the zeros of $\phi(\nu)$ at $z_j$ is also an appropriate choice in the case where $\phi(\nu)$ is given by the non-polynomial expresion specified in Definition 2.1. This assumption leads us to the system of equations [6]

$$\phi(z_j) = 0,\quad j = 1,...,q_0, \tag{2.16}$$

For (2.1) we obtain a *linear* system for the free parameters $\beta_{p+1},...,\beta_m$:

$$z_j + z_j^2\tan(z_j)\beta_2 - z_j^3\beta_3 - z_j^4\tan(z_j)\beta_4 + z_j^5\beta_5 + ... = \tan(z_j),\quad j = 1,...,m-p. \tag{2.17}$$

Evidently, the solution of this system converges to the values given in Table 2.1a as $h\to 0$.

For (2.4) a *nonlinear* system for the free $\sigma_j$ and $\pi_j$ is obtained:

$$[2-\sigma_1 z_j^2 + \sigma_2 z_j^4 - \sigma_3 z_j^6 + ...] = 2\cos(z_j)\sqrt{1-\pi_1 z_j^2 + \pi_2 z_j^4 - \pi_3 z_j^6 + ...},\quad j = 1,...,q_0. \tag{2.18}$$

Here, we have $\sigma_1 = 1$, $\pi_1 = 0$ for $p\geqslant 2$ and $\sigma_2 = 1/12$, $\pi_2 = 0$ for $p\geqslant 4$, etc. If we choose $P(z)\equiv 1$, i.e., $\pi_j = 0$, we have a *linear* system for the free $\sigma_j$.

## 3. CONSTRUCTION OF THE NUMERICAL METHODS

In this section the parameters $\lambda_{jl}$, $\mu_j$ and $\lambda'_l$ ocurring in (2.1) and (2.4) will be determined taking into account the consistency conditions and the dispersion relations listed in Table 2.1a and Table 2.2a.

*3.1 Runge-Kutta methods*

The various examples presented in this subsection will be given by means of the generating Butcher array

$$\begin{array}{c|c} \mu & L \\ \hline & \lambda^T \end{array} \qquad \mu := (\mu_j)_{j=1}^{m-1}, \quad L := (\lambda_{j,l})_{j,l+1=1}^{m-1}, \quad \lambda := (\lambda_{m,l})_{l=0}^{m-1} \tag{3.1}$$

In the examples we give the order $p$, the dispersion order $q$, with its error constant $c$, and the order of dissipation $r$. Furthermore, we compute the imaginary stability interval $(0,\beta)$, i.e., the interval where $|\tilde{a}(v)|<1$.

We have restricted our considerations to methods with $m \leqslant 6$ and $p = 2,3,4$. For $p = 4$ and $q>4$ the methods derived turned out to be unstable ($\beta = 0$) and are therefore omitted.

EXAMPLE 3.1. *A family of second order methods*

In [4, p.114] it was shown that the method generated by

$$\begin{array}{c|ccccc} \beta_m/\beta_{m-1} & \beta_m/\beta_{m-1} & & & & \\ \beta_{m-1}/\beta_{m-2} & 0 & \beta_{m-1}/\beta_{m-2} & & & \\ \vdots & \vdots & & \ddots & & \\ \beta_4/\beta_3 & & & & \beta_4/\beta_3 & \\ 2\beta_3 & 0 & \cdots & 0 & 2\beta_3 & \\ 1/2 & 0 & \cdots & 0 & 0 & 1/2 \\ \hline & 0 & \cdots & 0 & 0 & 0 \quad 1 \end{array} \tag{3.2}$$

is second order accurate for all values of $\beta_3, \beta_4, \ldots, \beta_m$. Solving the dispersion relations in Table 2.1a for $p = 2$ and $m = 4,5$ and 6 yields the methods

$$\begin{array}{c|ccccc} 1/5 & 1/5 & & & & \\ 1/3 & 0 & 1/3 & & & \\ 1/2 & 0 & 0 & 1/2 & & \\ \hline & 0 & 0 & 0 & 1 & \end{array} \qquad \begin{array}{l} p = 2, q = 6, r = 3 \\ c = -1/210 \\ (0,\beta)\approx(0,2.66) \end{array} \tag{3.3}$$

$$\begin{array}{c|ccccc} 1/8 & 1/8 & & & & \\ 8/35 & 0 & 8/35 & & & \\ 1/3 & 0 & 0 & 1/3 & & \\ 1/2 & 0 & 0 & 0 & 1/2 & \\ \hline & 0 & 0 & 0 & 0 & 1 \end{array} \qquad \begin{array}{l} p = 2, q = 8, r = 3 \\ c = -1/28350 \\ (0,\beta)\approx(3.38) \end{array} \tag{3.4}$$

$$\begin{array}{c|ccccc} 1/12 & 1/12 & & & & \\ 4/25 & 0 & 4/25 & & & \\ 5/21 & 0 & 0 & 5/21 & & \\ 1/3 & 0 & 0 & 0 & 1/3 & \\ 1/2 & 0 & 0 & 0 & 0 & 1/2 \\ \hline & 0 & 0 & 0 & 0 & 0 \quad 1 \end{array} \qquad \begin{array}{l} p = 2, q = 10, r = 3 \\ c = -1964/1091475 \\ (0,\beta)\approx(0,3.99) \end{array} \tag{3.5}$$

These methods are easily implemented and require only a few arrays for storage. Notice the relatively large (imaginary) stability intervals.

EXAMPLE 3.2 *A family of third order methods*

It was shown in [4, p.116] that the method

$$
\begin{array}{c|cccccc}
\lambda_1 & \lambda_1 & & & & & \\
\lambda_2 + 1/4 & 1/4 & \lambda_2 & & & & \\
\vdots & \vdots & & \ddots & & & \\
\lambda_{m-3} + 1/4 & 1/4 & & & \lambda_{m-3} & & \\
\lambda_{m-2} + 1/4 & 1/4 & 0 & \cdots & 0 & \lambda_{m-2} & \\
2/3 & 1/4 & 0 & \cdots & 0 & 0 & 5/12 \\
\hline
 & 1/4 & 0 & \cdots & 0 & 0 & 0 \quad 3/4
\end{array}
\tag{3.6}
$$

is third order accurate for all $\lambda_j$, $j = 1,...,m-3$, provided that $\lambda_{m-2} = 17/60 + \mathcal{O}(h)$. In terms of the parameters $\beta_j$ we have

$$\lambda_1 = \frac{\beta_m}{\beta_{m-1}}(1 + \frac{1}{4\lambda_2}),$$

$$\lambda_j = \frac{\beta_{m-j+1}}{\beta_{m-j}}(1 + \frac{1}{4\lambda_{j+1}}) - \frac{1}{4}, \quad j = 2,3,...,m-2,$$

where $\beta_3$ should satisfy the relation $\beta_3 = 1/6 + \mathcal{O}(h)$ as $h \to 0$.

By means of the dispersion relations the parameters $\beta_j$ can be found and on substitution the following three methods were constructed:

$$
\begin{array}{c|ccc}
32/85 & 32/85 & & \\
8/15 & 1/4 & 17/60 & \\
2/3 & 1/4 & 0 & 5/12 \\
\hline
 & 1/4 & 0 & 0 \quad 3/4
\end{array}
\qquad
\begin{array}{l}
p = 3, q = 6, r = 3 \\
c = -1/210 \\
(0,\beta) \approx (0,2.66)
\end{array}
\tag{3.7}
$$

$$
\begin{array}{c|cccc}
128/429 & 128/429 & & & \\
256/495 & 1/4 & 429/2380 & & \\
8/15 & 1/4 & 0 & 17/60 & \\
2/3 & 1/4 & 0 & 0 & 5/12 \\
\hline
 & 1/4 & 0 & 0 & 0 \quad 3/4
\end{array}
\qquad
\begin{array}{l}
p = 3, q = 8, r = 3 \\
c = -1/28350 \\
(0,\beta) \approx (0,3.38)
\end{array}
\tag{3.8}
$$

$$
\begin{array}{c|ccccc}
512/1899 & 512/1899 & & & & \\
512/1415 & 1/4 & 633/5660 & & & \\
160/357 & 1/4 & 0 & 283/1428 & & \\
8/15 & 1/4 & 0 & 0 & 17/60 & \\
2/3 & 1/4 & 0 & 0 & 0 & 5/12 \\
\hline
 & 1/4 & 0 & 0 & 0 & 0 \quad 3/4
\end{array}
\qquad
\begin{array}{l}
p = 3, q = 10, r = 3 \\
c = -1964/1091475 \\
(0,\beta) \approx (0,3.99)
\end{array}
\tag{3.9}
$$

Alternatively, we could have derived the parameters $\beta_j$ by solving the minimax relations (2.17). For instance, for $m = 4$ we find the method

$$
\begin{array}{c|ccc}
64\beta_4/(64\beta_3 - 5) & 64\beta_4/(64\beta_3 - 5) & & \\
16\beta_3/5 & 1/4 & (64\beta_3 - 5)/20 & \\
2/3 & 1/4 & 0 & 5/12 \\
\hline
 & 1/4 & 0 & 0 \quad 3/4
\end{array}
\tag{3.10a}
$$

where $\beta_3$ and $\beta_4$ are defined by

$$z_j + \frac{1}{2}z_j^2 \tan(z_j) - z_j^3\beta_3 - z_j^4 \tan(z_j)\beta_4 = \tan(z_j), \; j = 1,2; \tag{3.10b}$$

here, the $z_j$ are given by (2.15) for $q_0 = 2$. Since the solution for $\beta_3$ and $\beta_4$ converges to the values given in Table 2.1a ($p \geqslant 2$), we conclude that $\beta_3 \to 1/6$ as $h \to 0$ so that (3.10a) has the same $p, q$ and $r$ as (3.7).

*3.2. Runge-Kutta-Nyström methods*

The examples constructed below will be represented by the array

$$\begin{array}{c|c} \mu & L \\ \hline & \lambda^T \\ & \lambda'^T \end{array}, \quad \mu := (\mu_j)_{j=1}^{m-1}, \; L := (\lambda_{j,l})_{j,l+1=1}^{m-1},$$
$$\lambda := (\lambda_{m,l})_{l=0}^{m-1}, \; \lambda' := (\lambda'_l)_{l=0}^{m-1} \tag{3.11}$$

As before we give the orders $p, q$ and $r$, the error constant $c$ in the dispersion expansion, and the stability or periodicity intervals $(0,\beta)$ and $[0,\beta^2]$. We restrict our consideration to $m \leqslant 4$, $p = 2,3$ and zero-dissipative methods, that is $P(z) \equiv 1$.

EXAMPLE 3.3. *A family of second order methods with zero-dissipation*

Following [5] we consider methods generated by an array of the form

$$\begin{array}{c|cccc} \mu_1 & 0 & & & \\ \mu_2 & 0 & \lambda_{21} & & \\ \vdots & \vdots & & \ddots & \\ \mu_{m-2} & 0 & & & \lambda_{m-2,m-3} \\ 1/2 & 0 & \cdots & 0 & \lambda_{m-1,m-2} \\ \hline & 0 & & \cdots & 0 \quad 1/2 \\ & 0 & & \cdots & 0 \quad 1 \end{array} \tag{3.12}$$

This family of methods is second order accurate. If we set $P(z) \equiv 1$, then it can be shown that

$$\mu_j = \mu_1 = 1/2, \; \lambda_{j,j-1} = \frac{\sigma_{m-j+1}}{\sigma_{m-j}} = \frac{1}{(2m-2j+1)(2m-2j+2)}, \; j = 2,\ldots,m-1.$$

Below we give methods that are, respectively, dispersive of order $q = 4,6$ and 8, together with their intervals of periodicity $[0,\beta^2]$.

$$\begin{array}{c|ccc} 1/2 & 0 & & \\ 1/2 & 0 & 1/12 & \\ \hline & 0 & 0 & 1/2 \\ & 0 & 0 & 1 \end{array} \quad \begin{array}{l} [0,\beta^2] = [0,12] \approx [0,(3.46)^2] \\ c = 1/720 \\ p = 2, q = 4, r = \infty \end{array} \tag{3.13}$$

$$\begin{array}{c|ccc} 1/2 & 0 & & \\ 1/2 & 0 & 1/30 & \\ 1/2 & 0 & 0 & 1/12 \\ \hline & 0 & 0 & 0 \quad 1/2 \\ & 0 & 0 & 0 \quad 1 \end{array} \quad \begin{array}{l} [0,\beta^2] \approx [0,(2.75)^2] \\ c = -1/40320 \\ p = 2, q = 6, r = \infty \end{array} \tag{3.14}$$

$$
\begin{array}{c|ccccc}
1/2 & 0 & & & & \\
1/2 & 0 & 1/56 & & & \\
1/2 & 0 & 0 & 1/30 & & \\
1/2 & 0 & 0 & 0 & 1/12 & \\
\hline
 & 0 & 0 & 0 & 0 & 1/2 \\
 & 0 & 0 & 0 & 0 & 1
\end{array}
\qquad
\begin{array}{l}
[0,\beta^2]\approx[0,(4.63)^2] \\
c = 1/3628800 \\
p = 2, q = 8, r = \infty
\end{array}
\tag{3.15}
$$

EXAMPLE 3.4. *A third-order method with zero dissipation*

By solving numerically the consistency conditions for third order accuracy under the by-conditions of sixth order dispersion and $P(z)\equiv 1$, we found the following method

$$
\begin{array}{l|lll}
.926590210660 & .429284709246 & & \\
.421787206165 & .048227503064 & .040724720578 & \\
\hline
 & .233566863436 & .107544087262 & .158889049302 \\
 & .127854313973 & .261765691855 & .610379994172
\end{array}
\tag{3.16}
$$

where

$$p = 3, q = 6, r = \infty; c = -1/40320 \text{ and } [0,\beta^2] = [0,(2.75)^2].$$

## 4. NUMERICAL EXPERIMENTS

In this section we show that the methods derived in the preceding section on the basis of the test equation (1.2), may also be superior to conventional methods in nonmodel problems.

### *4.1 First order equations*

**Problem 4.1.** *Hyperbolic equation*

$$
\begin{aligned}
&\frac{\partial u}{\partial t} = -\frac{\partial u}{\partial x}, \quad 0 \leqslant x \leqslant 1, \, t \geqslant 0, \\
&u(t,0) = 0, \quad u(0,x) = \sin(\pi^2 x^2).
\end{aligned}
\tag{4.1}
$$

Discretization of $\partial/\partial x$ by symmetric differences at internal grid points and one-sided differences at the boundary point $x = 1$ yields the system

$$
\frac{dy}{dt} = \frac{1}{2\Delta x}
\begin{bmatrix}
0 & -1 & & & \\
1 & 0 & -1 & & \\
 & \ddots & \ddots & \ddots & \\
 & & 1 & 0 & -1 \\
 & & -1 & 4 & -3
\end{bmatrix} y.
\tag{4.2}
$$

In order to test the capability of the various methods to stay in phase with the exact solution, we have concentrated on approximating the zeros of the solution $y$. By choosing $\Delta x = 1/50$, we found that the 20-th component of the exact solution vector $y$ reaches its 500-th zero at the point

$$Z_{500} = 33.509996948\cdots. \tag{4.3}$$

Its numerical approximation $z_{500}$ was obtained by integrating with fixed step size and by applying cubic spline interpolation based on 10 neighbouring step points $t_n = t_0 + nh$, where $h$ is the step size in the experiment under consideration. The accuracy of this approximation, relative to the distribution of the successive zeros on the $t$-axis, was measured by the value of

$$sd := -\log_{10}\left|\frac{Z_{500}-z_{500}}{Z_{501}-Z_{500}}\right|, \tag{4.4}$$

TABLE 4.1. Relative errors in computing (4.3)

| method | p/q | h | sd | h | sd | h | sd |
|---|---|---|---|---|---|---|---|
| RK4 | 4/4 | 1/90 | −.37 | 1/180 | 1.61 | 1/270 | 2.31 |
| (3.3) | 2/6 | 1/90 | −.33 | 1/180 | 3.30 | 1/270 | 4.12 |
| (3.4) | 2/8 | 1/72 | −.33 | 1/144 | 3.98 | 1/216 | 4.41 |
| (3.5) | 2/10 | 1/60 | −.33 | 1/120 | 3.99 | 1/180 | 4.65 |
| (3.7) | 3/6 | 1/90 | −.33 | 1/180 | 3.30 | 1/270 | 4.12 |
| (3.8) | 3/8 | 1/72 | −.33 | 1/144 | 3.98 | 1/216 | 4.41 |
| (3.9) | 3/10 | 1/60 | −.33 | 1/120 | 3.99 | 1/180 | 4.65 |

where $Z_{501}$ denotes the 501-st zero of the solution $y^{(20)}$.

In Table 4.1 the sd-values obtained by the various methods constructed in Section 3.1 are listed, together with the results produced by the conventional, standard fourth-order method *RK*4. The integration steps were chosen such that all results listed in one column require the same number of right-hand side evaluations.

The results in Table 4.1 clearly demonstrate that the accuracy is mainly determined by the order of dispersion $q$ and is independent of the algebraie order $p$.

*4.2 Second order equations*

**Problem 4.2.** *Wave equation*

$$\frac{\partial^2 u}{\partial t^2} = gd(x)\frac{\partial^2 u}{\partial x^2} + \frac{1}{4}\lambda^2(x,u)u,\ 0 \leqslant x \leqslant b,\ t \geqslant 0$$

$$\frac{\partial u}{\partial x}(t,0) = \frac{\partial u}{\partial x}(t,b) = 0, \tag{4.5}$$

$$u(0,x) = \sin(\frac{\pi x}{b}),\quad \frac{\partial u}{\partial t}(0,x) = -\frac{\pi}{b}\sqrt{gd}\ \cos(\frac{\pi x}{b})$$

Here, $d(x)$ is the depth function given by $d = d_0[2 + \cos(2\pi x / b)]$, $g$ denotes the acceleration of gravity, and $\lambda(x,u)$ is the coefficient of bottom friction defined by $\lambda = g\,|u|\,/\,C^2 d$ with Chezy coefficient $C$.

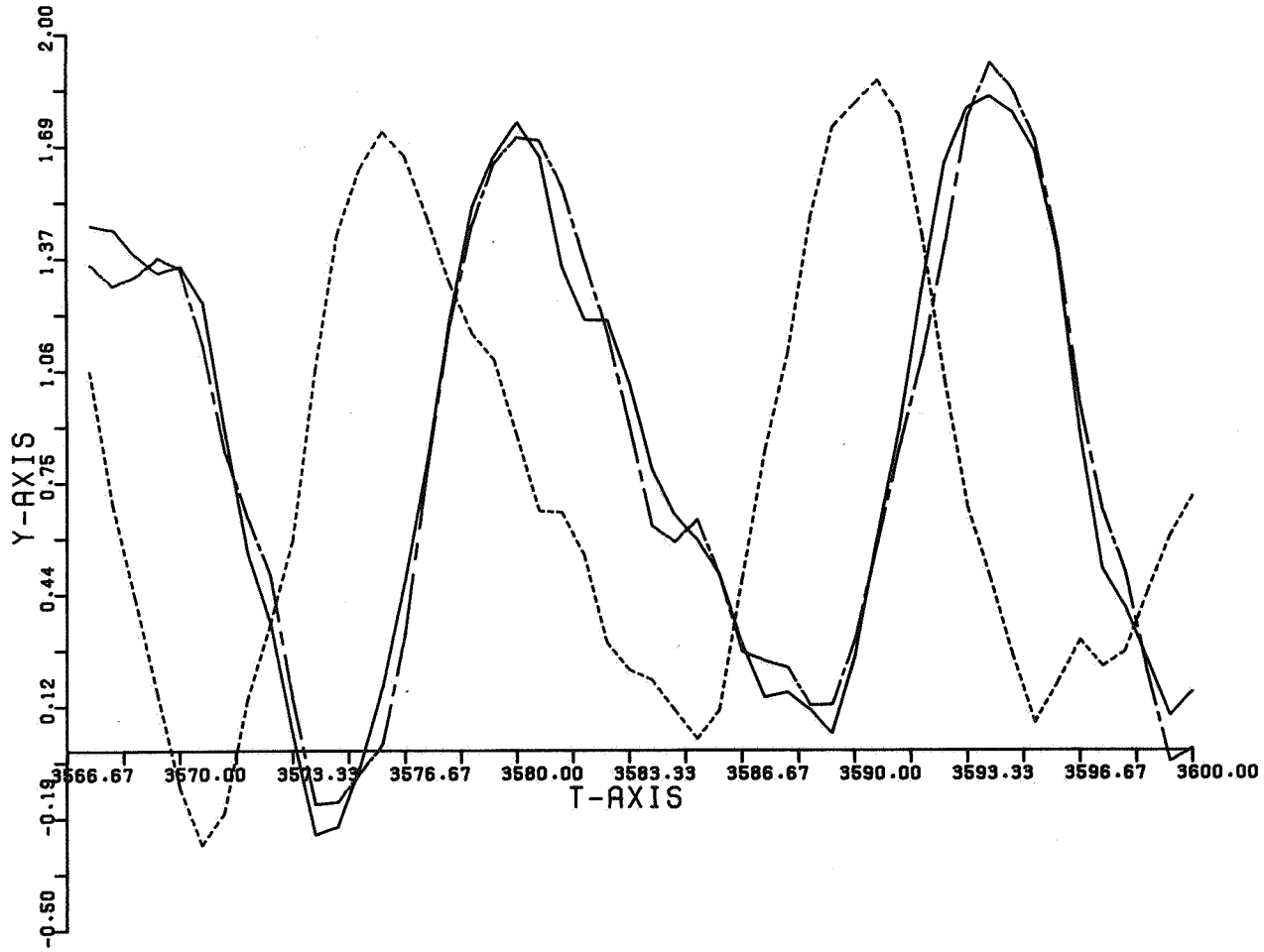


FIGURE 4.1. exact solution (——) of problem (4.5) and the solutions obtained by the Runge-Kutta-Nyström method (3.13) (—·—) and by the Störmer method (— — — —).

By using second-order symmetric differences, this problem was converted into a system of ODEs, and integrated by method (3.13) and by the well-known second-order, explicit Störmer method (see eg. [7, p.260]). Figure 4.1 shows the results in the interval $3567 < t \leqslant 3600$, in the case where

$$\Delta x = 10,\ b = 100,\ g = 9.81,\ d_0 = 10,\ C = 50;$$

the step size $h$ was such that both experiments required the same number of right-hand side evaluations.

Again, the superiority of the high-order dispersive method (3.13) is clear.

**Problem 4.3.** *Bessel equation*

$$\frac{d^2y}{dt^2} = -(100 + \frac{1}{4t^2})y,\ t \geqslant 1$$

$$y(t) = \sqrt{t}J_0(10t). \tag{4.6}$$

In order to show that high-order dispersive methods are suitable for long interval integration, we have applied the conventional fourth-order Nyström method and the methods constructed in Section 3.2 on relatively large integration intervals. As before, all experiments required the same computational effort. The accuracy was measured by

$$sd(T) := -\log_{10}\Big(\max_{\substack{t_n=1+nh \\ n=1,\ldots,(T-1)/h}} |y(t_n)-y_n|\Big) \tag{4.7}$$

and its value, produced by the various methods, is listed in Table 4.2.

TABLE 4.2. The maximal absolute error (4.7) for equation (4.6)

| method | h | m | p | q | r | s | sd(100) | sd(500) | sd(1000) | sd(4000) |
|---|---|---|---|---|---|---|---|---|---|---|
| Nyström | 1/20 | 3 | 4 | 4 | 5 | 4 | 1.3 | .7 | .5 | .4 |
| (3.13) | 1/30 | 2 | 2 | 4 | ∞ | 2 | 2.4 | 1.7 | 1.4 | .8 |
| (3.14) | 1/20 | 3 | 2 | 6 | ∞ | 2 | 2.9 | 2.8 | 2.7 | 2.3 |
| (3.15) | 1/15 | 4 | 2 | 8 | ∞ | 2 | 2.7 | 2.7 | 2.7 | 2.7 |
| (3.16) | 1/20 | 3 | 3 | 6 | ∞ | 3 | 3.2 | 3.2 | 3.2 | 2.5 |

It turned out that the Nyström method missed a few zeros when applied on the intervals [1,1000] and [1,4000] whereas the high-order dispersion method found the correct number of zeros in all experiments. Moreover, this Table clearly shows that the methods with a relatively low order of dispersion gradually loose accuracy, whereas for method (3.15), having $q = 8$, the accumulation of phase errors is not yet visible on these time-intervals.

**Problem 4.4.** *Inhomogeneous equation*

$$\frac{d^2y}{dt^2} = -\omega^2 y + (\omega^2-1)\sin(t),\ t \geqslant 0 \tag{4.8}$$

$$y(t) = \cos(\omega t) + \sin(\omega t) + \sin(t),\ \omega >> 1.$$

We conclude this paper with an experiment on the inhomogeneous equation (4.8) whose exact solution consists of a rapidly and a slowly oscillating function; the slowly varying function is due to the inhomogeneous term. The purpose is to show that high-order dispersive methods are able to integrate this problem with relatively large integration steps (i.e., $\omega h$ not small), because the high-order dispersion will take care for the rapidly oscillating component and the algebraic order, although modest, will take care for the slowly varying component.

Table 4.3 presents the analogue of Table 4.2 for equation (4.8).

TABLE 4.3. The maximal absolute error (4.7) for equation (4.8) with $\omega = 10$

| method | h | m | p | q | r | s | sd(100) | sd(500) | sd(1000) | sd(4000) |
|---|---|---|---|---|---|---|---|---|---|---|
| Nyström | 1/20 | 3 | 4 | 4 | 5 | 4 | .6 | −.1 | −.3 | −.3 |
| (3.13) | 1/30 | 2 | 2 | 4 | ∞ | 2 | 1.7 | .9 | .6 | .0 |
| (3.14) | 1/20 | 3 | 2 | 6 | ∞ | 2 | 1.7 | 1.6 | 1.6 | 1.4 |
| (3.15) | 1/15 | 4 | 2 | 8 | ∞ | 2 | 1.4 | 1.4 | 1.4 | 1.4 |
| (3.16) | 1/20 | 3 | 3 | 6 | ∞ | 3 | 2.7 | 2.7 | 2.4 | 1.7 |

Again the Nyström method did not find the correct number of zeros on the intervals [0,1000] and [0,4000]: it missed about 10% and 50% of the zeros on these intervals. The other methods did find them all. The sd-values as given in the Table, show the same tendency as was mentioned in the previous example.

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# Appendix

In the course of this investigation of Runge-Kutta (-Nyström) methods, we constructed many other methods. A few of them are listed in this appendix, because they might become of interest in our future research in this area. They are all of Runge-Kuta-Nyström type, they are dissipative, and they have an increased order of dispersion.

*A family of second-order, dissipative methods*

We again consider methods generated by an array of the form (3.11), but now we exploit the polynomial $P(z)$ in order to increase the order of dispersion. By solving the dispersion relations listed in Table 2.2a we find the optimal parameters $\sigma_j$ and $\pi_j$. The Runge-Kutta-Nyström parameters, expresed in terms of $\sigma_j$, are then given by (cf. [5])

$$\mu_j = \frac{1}{2}\,\frac{\sigma_{m-j} + \pi_{m-j}}{\sigma_{m-j} - \pi_{m-j}}, \quad \lambda_{j,j-1} = \frac{\sigma_{m-j+1} - \pi_{m-j+1}}{\sigma_{m-j} - \pi_{m-j}}, \; j = 1,\ldots,m-1,$$

where $\sigma_1 = 1$ and $\sigma_m = \pi_1 = \pi_m = 0$.

In the special cases given below we have added the stability interval $(0,\beta)$, that is, the interval $0<\nu<\beta$ where $|\tilde{a}_{\pm}(\nu)|<1$.

$$\begin{array}{c|ccc} 13/30 & 0 & & \\ 1/2 & 0 & 1/12 & \\ \hline & 0 & 0 & 1/2 \\ & 0 & 0 & 1 \end{array} \qquad \begin{array}{l} p = 2, q = 6, r = 3 \\ (0,\beta) = (0,\sqrt{12}) \approx (0,3.46) \end{array} \tag{A1}$$

$$\begin{array}{c|cccc} .266830712 & 0 & & & \\ .065635306 & 0 & -.183849014 & & \\ 1/2 & 0 & 0 & 1/12 & \\ \hline & 0 & 0 & 0 & 1/2 \\ & 0 & 0 & 0 & 1 \end{array} \qquad \begin{array}{l} p = 2, q = 10, r = 3 \\ (0,\beta) \approx (0,2.40) \end{array} \tag{A2}$$

Here,

$$\sigma_1 = 1, \; \sigma_2 = .04713627554, \; \sigma_3 = -.01174842249$$

$$\pi_1 = 0,\ \pi_2 = -.03619705780,\ \pi_3 = .00357232863.$$

*Some higher order methods*

Our starting point for the construction of third- and fourth- order methods is a *full* parameter matrix with $m = 3$ and 4, respectively. In order to achieve an order of dispersion as high as possible we only consider the case where $P(z) \neq 1$. We no longer follow the analytical approach, as was possible in section 3.2 section, but we formulate a minimization problem for a nonlinear least-squares problem of the form

$$G(\Lambda) = \sum_i [g_i(\Lambda)]^2$$

in which $\Lambda$ denotes the vector of all RKN parameters and $g_i$ stands for the consistency- and dispersion-relations. Moreover, we added to this system an extra $g$-function of the form $g(\Lambda) = W / \beta(\Lambda)$, where $\beta$ denotes the stability boundary and $W$ is some weight. For the minimization of $G(\Lambda)$ we used the NAG-routine EO4FCF. We found the following three-stage *third-order* RKN schemes:

$$\begin{array}{l|lll} .4969003529 & .1234549803 & & \\ .7337223214 & .1504173630 & .1187568595 & \\ \hline & .2260389606 & .1450231299 & .1289379095 \\ & .2265821428 & .2849142164 & .4885036408 \end{array} \tag{A3}$$

which is of dispersion order $q = 8$, of dissipation order $r = 3$ and has $\beta = 4.56$, and

$$\begin{array}{l|lll} .4955018983 & .1227610656 & & \\ .7166211542 & .1493614124 & .1074115269 & \\ \hline & .2280103951 & .1277448126 & .1442447923 \\ & .2319401058 & .2279673366 & .5400925576 \end{array} \tag{A4}$$

which has $q = 10$, $r = 3$ and $\beta = 3.12$.

The least-squares approach allows us to impose more (dispersion) relations than the number of free parameters. In this way we found a scheme which is *effectively* of order $q = 12$, $r = 3$, that is the "residuals" $g_i$ are sufficiently small. This scheme reads

$$\begin{array}{l|lll} .4940895709 & .1220622521 & & \\ .7075002625 & .1489112009 & .1013671098 & \\ \hline & .2296630303 & .1152557560 & .1550812137 \\ & .2348807666 & .1936269363 & .5714922971 \end{array} \tag{A5}$$

The interval of stability is given by (0, 3.07).

Proceeding in the same way, *fourth-order* schemes were constructed. As an example, we give a scheme which has $q = 10$ and $r = 5$:

$$\begin{array}{l|llll} .0551594317 & .0015212815 & & & \\ .6683701446 & -1.1732016116 & 1.3965609367 & & \\ .3632109628 & 1.5887403855 & -1.7263289145 & .2035496308 & \\ \hline & .4046440250 & -.3464696799 & .0829134999 & .3589121550 \\ & -1.8067389251 & 2.6410990864 & .9639436971 & -.7983038584 \end{array} \tag{A6}$$

Its stability interval is (0, 3.59).