

EXPLICIT RUNGE-KUTTA (-NYSTRÖM) METHODS WITH REDUCED PHASE ERRORS FOR COMPUTING OSCILLATING SOLUTIONS*

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Abstract. 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 equations describing free and weakly forced oscillations and to semidiscretized hyperbolic equations reveals that the phase errors can significantly be reduced.

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

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1. Introduction. We shall discuss the construction of special Runge-Kutta (-Nyström) methods (RK(N) methods) for integrating systems of ODEs of the form

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

The methods are designed in such a way that for *linear* systems with $f(t, y) = Ay + g(t)$, where A is skew symmetric if $k = 1$ and symmetric if $k = 2$, the phase error of the free oscillations in the numerical solution is small. Methods possessing this property are suitable for long interval integration of equations describing *free oscillations* because the integration step can be chosen much larger than the step size conventional RK(N) methods need for the accurate representation of these components (see the numerical results for Problem 4.3). A second class of problems which can efficiently be integrated by these methods, have solutions that consist of *free oscillations of high frequency and forced oscillations of low frequency* (see Problem 4.4). Since the step size needs only to be tuned to the forced oscillation, the method can again be applied with relatively large steps. In all other cases, the efficiency of the methods depends on the magnitude of the phase error due to the forced oscillations. If these contributions are small, for example, if $|g(t)| \ll |Ay(t)|$, then the methods derived in this paper are still more efficient than conventional RK(N) methods (see Problem 4.5). Because the classes of problems described above are usually not stiff, we shall confine our considerations to *explicit* methods (although the process of reducing the phase error of the method could be extended to implicit RK(N) methods). Finally, we mention another class of problems for which these explicit methods may prove to be suitable, namely the class of *semidiscrete hyperbolic equations with smooth solutions*. The introduction of vector computers stimulated a reconsideration of explicit time-stepping methods for solving hyperbolic equations (see, e.g., Jameson [14]) because on this new generation of computers, explicit methods can be implemented with great efficiency, partly compensating for the limited step size inherent to explicit methods.

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With this second application in mind, we have constructed the RK(N) methods in such a way that a minimum of intermediate storage is required, so that large systems of semi-discrete hyperbolic equations can be handled.

Most papers devoted to the phase lag analysis of numerical methods start with the inhomogeneous test equation

$$(1.2) \quad \frac{d^k y}{dt^k} = (i\omega)^k y + c e^{i\omega_p t}, \quad \omega, \omega_p, c \in \mathbb{R}.$$

The exact solution of this equation is given by

$$(1.3) \quad y(t) = c_+ e^{i\omega t} + c_- e^{-i\omega t} + \frac{c}{(i\omega_p)^k - (i\omega)^k} e^{i\omega_p t},$$

where c_+ and c_- are constants with $c_- = 0$ for $k = 1$. By applying a numerical method to the test equation (1.2) and assuming that the characteristic polynomial characterizing the method has d distinct zeros $\{\tilde{a}_j\}$ (so-called *amplification factors*), we find for the numerical approximation at $t_n = nh$ an expression of the form

$$(1.4) \quad y_n = \sum_{j=1}^d \tilde{c}_j (\tilde{a}_j(\omega h))^n + ch^k \tilde{\Omega}(\omega h, \omega_p h) e^{i\omega_p h},$$

where the constants \tilde{c}_j are determined by the initial conditions, and where the functions \tilde{a}_j and $\tilde{\Omega}$ are independent of n and are completely determined by the numerical method applied. The functions $(\tilde{a}_j)^n$ and $\tilde{\Omega}$ are discrete analogues of the functions $\exp(\pm i\omega t)$ and $\Omega := 1/[(i\omega_p h)^k - (i\omega h)^k]$. Accordingly, the functions $ch^k \Omega \exp(i\omega_p h)$ and $ch^k \tilde{\Omega} \exp(i\omega_p h)$ will be called the inhomogeneous solution components of the exact and of the numerical solution, respectively.

For example, if Euler's method is applied to (1.2) with $k = 1$, we obtain

$$d = 1, \quad \tilde{a}^n = [1 + i\omega h]^n, \quad \tilde{\Omega} = \frac{1}{(e^{i\omega_p h} - 1) - (i\omega h)}.$$

In the phase analysis of the *homogeneous* components of the exact solution (1.3) and the numerical solution (1.4), one compares the phase(s) (or argument(s)) of $\exp(\pm i\omega h)$ with the phase(s) of the *principal* characteristic root(s) occurring in the set $\{\tilde{a}_j\}$. Likewise, the phase analysis of *inhomogeneous* solution components is based on the phases of the functions Ω and $\tilde{\Omega}$. In this connection it should be observed that the "inhomogeneous" phase error (due to differing phases of Ω and $\tilde{\Omega}$) is constant in time, whereas the "homogeneous" phase errors are time-dependent and must accumulate as n increases.

In the case of first-order equations ($k = 1$), a complete phase analysis has been carried out by Brusa and Nigro [2] for a special third-order implicit one-step method, and for second-order equations ($k = 2$), a phase-lag analysis may be found in Gladwell and Thomas [8] for linear multistep methods and in Thomas [20] for certain hybrid families related to the multistep Runge-Kutta methods of Cash [3] and Chawla [4]. The papers mentioned above treat both the *homogeneous* and *inhomogeneous* components in the phase error. In Strehmel [19] and Strehmel and Weiner [18], *inhomogeneous* phase errors are investigated for Rosenbrock-type methods (adaptive Runge-Kutta-Nyström methods). This analysis is extended to explicit Runge-Kutta-Nyström methods and to predictor-corrector methods in van der Houwen, Sommeijer, Strehmel and Weiner [13]; an analysis of the *homogeneous* phase errors for Numerov-type methods is given by Chawla et al. [5], [6], for multiderivative methods by Twizell

[22] and Twizell and Khaliq [21] and for predictor-corrector-type methods in van der Houwen and Sommeijer [12].

Since we shall confine our considerations to homogeneous phase errors we will use the test equation

$$(1.5) \quad \frac{d^k y}{dt^k} = (i\omega)^k y, \quad \omega \text{ real.}$$

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. Methods of (algebraic) order 2 and 3, and of dispersion order up to 10 will be derived. We emphasize that, whereas the algebraic order applies to ODEs of the general form (1.1), the order of dispersion only applies to equations of the homogeneous form: $f(t, y) = Ay$, where A has eigenvalues $(i\omega)^k$, ω real. However, as outlined above, in the case of inhomogeneous problems, an increased order of (homogeneous) dispersion may improve the overall accuracy considerably, although numerical results will show the algebraic order and not the dispersion order.

In addition to RK(N) methods with fixed coefficients, we shall shortly discuss a simple modification in which the coefficients can be tuned to exploit possible extra information available on the dominant frequencies in the exact solution. These modified methods are related to the oscillatory RK methods proposed by Bettis [1], but they have the advantage of being less sensitive to errors in the estimation of the dominant frequencies (see § 2.5 and Problem 4.3).

Finally, a few comments on the actual implementation of the RK(N) methods. The implementation of such a method itself is extremely simple, because of its explicit structure. However, to run these methods efficiently on a computer, a step size strategy is required, not only to monitor the (local) accuracy of the numerical solution, but also to avoid the development of instabilities due to step sizes violating the stability condition inherent to explicit methods (when a fixed step implementation is used, an estimate of the spectral radius of the Jacobian matrix $\partial f/\partial y$ of (1.1) should be provided in order to satisfy the stability condition $h < \beta/\text{spectral radius}$, where β is the imaginary stability boundary (see § 3)). Usually, step size control for RK(N) methods is based on embedded pairs of methods, providing both a numerical solution and a reference solution. As the referees of this paper observed, the order properties of the main formula and of the reference formula would have to be carefully matched to obtain a good local error estimate. The systematic construction of such reference formulas for our RK(N) methods is not discussed in this paper. However, in § 3.1 an illustration of the construction of a reference formula is given.

2. Dispersion and dissipation in Runge–Kutta (–Nyström) 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

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

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 (1.5) with $k = 1$ yields the numerical solution

$$(2.2) \quad y_n = \tilde{a}^n y_0, \quad \tilde{a} := A_m(\nu^2) + i\nu B_m(\nu^2), \quad \nu := \omega h,$$

where A_m and B_m are polynomials in ν^2 , completely defined by the Runge-Kutta parameters $\lambda_{j,l}$; $\tilde{a} = \tilde{a}(\nu)$ will be called the *amplification factor*. A comparison of (2.2) with the solution of (1.5), i.e. $y(t_n) = y_0 \exp(in\nu)$, leads us to the following definition:

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

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

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

It follows from (2.2) that

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

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

$$(2.4) \quad \begin{aligned} y_n^{(0)} &= y_{n-1}, \\ y_n^{(j)} &= y_{n-1} + \mu_j h \dot{y}_{n-1} + h^2 \sum_{l=0}^{j-1} \lambda_{j,l} f(t_{n-1} + \mu_l h, y_n^{(l)}), \quad j = 1, \dots, m, \\ y_n &:= y_n^{(m)}, \quad \dot{y}_n := \dot{y}_{n-1} + h \sum_{l=0}^{m-1} \lambda_l f(t_{n-1} + \mu_l h, y_n^{(l)}), \end{aligned}$$

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

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

where A_m, A_m^*, B_m and B_m^* are again polynomials in ν^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

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

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

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

We compare this discrete solution with the continuous solution

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

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

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

and similarly

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

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

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

$$(2.6') \quad y(t_n) = 2|c| \cos(\psi + n\nu).$$

These expressions lead us to the following definition.

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

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

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

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 $O(\nu^s)$ then the initial dispersion and initial amplification error are both $O(\nu^s)$ as $\nu \rightarrow 0$. 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 $\phi(\nu)$ and $\alpha(\nu)$ 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 $\phi(\nu)$ and $\alpha(\nu)$ defined in Definition 2.1.) It follows from (2.5) that

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

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 $\phi(\nu) = O(\nu^{q+1})$). 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

$$(2.8) \quad A_m(z) = 1 - \beta_2 z + \beta_4 z^2 \cdots, \quad B_m(z) = 1 - \beta_3 z + \beta_5 z^2 \cdots,$$

where $\beta_j = 0$ for $j > m$. We want to express the conditions for dispersion of order q in terms of the parameters $\beta_j, j = 2, \dots, m$ (in the Appendix, we give a few of these β_j -coefficients explicitly expressed in terms of the parameters of the RK scheme (2.1)).

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

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

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

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

and

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

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

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

then

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

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). \square

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

$$(2.10) \quad \beta_j = \frac{1}{j!}, \quad j = 2, \dots, p.$$

Hence, an m -stage, p th order method has $m - p$ free parameters β_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 $\beta_{p+1}, \dots, \beta_m$ 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. \square

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.

2.3. Runge-Kutta-Nyström methods with zero dissipation. We shall say that a Runge-Kutta-Nyström method has *zero dissipation* at a point ν if $\alpha(\nu) = 0$ where $\alpha(\nu)$

TABLE 2.1a
Dispersion relations in terms of the parameters β_j .

Order	$q \cong$
$p = 1$	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 $62\beta_2 - 153\beta_4 + 378\beta_6 - 945\beta_8 + 2835(\beta_{10} - \beta_{11}) = 1382/55$
$p = 2, 3$	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 2.1b
Error constants c in the dispersion $\phi(\nu) = c\nu^{q+1} + O(\nu^{q+3})$.

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	$-\beta_9 + \beta_8 - \frac{1}{3}\beta_6 + 2\beta_4/15 - 17\beta_2/315 + 62/2835$
10	$\beta_{11} - \beta_{10} + \frac{1}{3}\beta_8 - 2\beta_6/15 + 17\beta_4/315 - 62\beta_2/2835 + 1382/155925$
12	$-\beta_{13} + \beta_{12} - \frac{1}{3}\beta_{10} + 2\beta_8/15 - 17\beta_6/315 + 62\beta_4/2835 - 1382\beta_2/155925 + 21844/6081075$

is defined in Definition 2.2; thus, the numerical solution of our test equation, specified in (2.5''), assumes the form $y_n = 2|\tilde{c}| \cos(\tilde{\psi} + n\tilde{\nu})$. 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 $\{(1.5), k = 2\}$. The interval $0 \leq \nu^2 \leq \beta^2$ 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 nonempty 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

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

The analogue of Theorem 2.1 becomes the following.

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

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

Then the method is dispersive of order $q = 2q_0$ if the parameters σ_j are given by

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

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

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

Hence,

$$\begin{aligned} \phi(\nu) &= \nu - \arccos \left(\frac{2 \cos(\nu) + O(\nu^{2q_0+2})}{2\sqrt{P(\nu^2)}} \right) \\ &= \nu - \arccos(\cos(\nu) + O(\nu^{q+2})) = O(\nu^{q+1}). \quad \square \end{aligned}$$

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 coincides with the dispersion relations (cf. (2.9)).

2.4. Dissipative Runge-Kutta-Nyström methods. By dropping the condition of periodicity intervals, the order of dispersion can be increased. Writing

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

and proceeding as in § 2.2, we arrive at the dispersion relations listed in Table 2.2a (the expressions for a few σ_j and π_j coefficients in terms of the parameters of the RKN scheme, can be found in the Appendix). We observe that in a p th order method the amplification factors \tilde{a}_\pm satisfy the relation

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

so that

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

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

TABLE 2.2a
Dispersion relations in terms of the parameters σ_j and π_j .

Order	$q \cong$
$p = 1$	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 $630\sigma_3^2 + 2520\sigma_6 + 1260\sigma_5 + 105\sigma_4 - 112\pi_3 - 840\pi_4 - 2520\pi_5 - 2520\pi_6 = 16/1485$

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

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 $[\underline{\nu}, \bar{\nu}] := [\underline{\omega}h, \bar{\omega}h]$. If $\phi(\nu)$ were a *polynomial*, then this minimax problem could be solved by resorting to the celebrated Chebyshev theorem: "Of all monic polynomials of degree m on the interval $[\underline{\nu}, \bar{\nu}]$, the shifted and (scaled) Chebyshev polynomial $T_m(x)$ has the smallest maximum norm." Since $\phi(\nu)/\nu$ is an *even* function, this theorem suggests the identification of $\phi(\nu)/\nu$ with a Chebyshev polynomial in ν^2 shifted to the interval $[\underline{\nu}, \bar{\nu}]$. Such an identification is accomplished by assigning to $\phi(\nu)$ the same zeros as this shifted Chebyshev polynomial possesses, i.e. the zeros

$$(2.15) \quad z_j := \left[\frac{1}{2} \bar{\nu}^2 + \frac{1}{2} \underline{\nu}^2 + \frac{1}{2} (\bar{\nu}^2 - \underline{\nu}^2) \cos \left(\frac{2j-1}{2q_0} \pi \right) \right]^{1/2}, \quad j = 1, \dots, q_0,$$

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 nonpolynomial expression specified in Definition 2.1. This assumption leads us to the system of equations [11]:

$$(2.16) \quad \phi(z_j) = 0, \quad j = 1, \dots, q_0.$$

For the Runge-Kutta methods we obtain a *linear* system for the free parameters $\beta_{p+1}, \dots, \beta_m$:

$$(2.17) \quad z_j + z_j^2 \tan(z_j)\beta_2 - z_j^3\beta_3 - z_j^4 \tan(z_j)\beta_4 + z_j^5\beta_5 + \dots = \tan(z_j), \quad j = 1, \dots, q_0.$$

For the Runge-Kutta-Nyström methods a *nonlinear* system for the free σ_j and π_j is obtained:

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

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

In cases where it is known in advance that given frequencies $\omega_1, \omega_2, \dots$ are dominating in the exact solution, we can directly put $z_j = \omega_j h$. The resulting method integrates the corresponding oscillations exactly and is, when only one frequency ω_1 is involved, identical to the oscillatory RK methods proposed by Bettis [1]. This approach can be compared with an analogous technique proposed by Gautschi [7] to increase the so-called trigonometric order of linear multistep methods. A disadvantage of both the Gautschi and Bettis methods is the sensitivity to an inaccurate estimate of the frequencies ω_j (compare the discussion in Neta and Ford [15] and in van der Houwen and Sommeijer [11]).

Finally, we remark that for $z_j \rightarrow 0, j = 1, \dots, q_0$, the solution of the systems (2.17) and (2.18) converge to the values given in the Tables 2.1a and 2.2a, respectively.

3. Construction of the numerical methods. In this section the parameters λ_{jl}, μ_j and λ'_l occurring 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

$$(3.1) \quad \frac{\mu}{\lambda} \Big| \frac{L}{\tau}, \quad \mu := (\mu_j)_{j=1}^{m-1}, \quad L := (\lambda_{j,l})_{j,l=1}^{m-1}, \quad \lambda := (\lambda_{m,l})_{l=0}^{m-1}.$$

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 $|\tilde{a}(\nu)| < 1$.

We have restricted our considerations to methods with $m \leq 6$ 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 [9, p. 114] it was shown that the method generated by

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

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

$$(3.3) \quad \begin{array}{c|cccc} 1/5 & 1/5 & & & \\ 1/3 & 0 & 1/3 & & \\ 1/2 & 0 & 0 & 1/2 & \\ \hline & 0 & 0 & 0 & 1 \end{array} \quad \begin{array}{l} p=2, \quad q=6, \quad r=3, \\ c=-1/630, \\ (0, \beta) \approx (0, 2.66), \end{array}$$

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

$$(3.5) \quad \begin{array}{c|cccccc} 1/12 & 1/12 & & & & \\ 4/25 & 0 & 4/25 & & & \\ 5/21 & 0 & 0 & 5/21 & & \\ 1/3 & 0 & 0 & 0 & 1/3 & \\ 1/2 & 0 & 0 & 0 & 0 & 1/2 \\ \hline & 0 & 0 & 0 & 0 & 0 & 1 \end{array} \quad \begin{array}{l} p=2, \quad q=10, \quad r=3, \\ c=-1/2182950, \\ (0, \beta) \approx (0, 3.99). \end{array}$$

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

Example 3.2. Construction of reference methods. In order to illustrate the construction of a reference method for use in step size control, we derive an RK method which can be used in combination with (3.3) for computing an estimate of the local error. Consider the method generated by the Butcher array

$$\begin{array}{c|cccccc} 1/5 & 1/5 & & & & \\ 1/3 & 0 & 1/3 & & & \\ 1/2 & 0 & 0 & 1/2 & & \\ 1 & 0 & 0 & 0 & 0 & 1 \\ \hline & \lambda_0 & \lambda_1 & \lambda_2 & \lambda_3 & \lambda_4 \end{array},$$

where the parameters $\lambda_0, \dots, \lambda_4$ are to be determined in such a way that this method is more accurate than (3.3). Since only one additional right-hand side evaluation is required when used together with (3.3), it is a good starting point for deriving a

relatively cheap reference formula. Notice that (3.3) is embedded in the reference formula. This formula should at least have order $p = 2$, i.e., we require

$$\beta_1 := \lambda_0 + \lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 = 1,$$

$$\beta_2 := \frac{1}{5}\lambda_1 + \frac{1}{3}\lambda_2 + \frac{1}{2}\lambda_3 + \lambda_4 = \frac{1}{2}.$$

Suppose that we want the method to have dispersion order $q = 8$. It then follows from Table 2.1a that, in addition, we should require

$$\beta_3 := \frac{1}{15}\lambda_2 + \frac{1}{6}\lambda_3 + \frac{1}{2}\lambda_4 = \frac{1}{6},$$

$$\beta_4 := \frac{1}{30}\lambda_3 + \frac{1}{6}\lambda_4 = \frac{4}{105}, \quad \beta_5 := \frac{1}{30}\lambda_4 = \beta_4 - \frac{1}{30}.$$

Solving these equations together with the ($p = 2$)-order conditions yields

$$\lambda_0 = -\frac{1}{21}, \quad \lambda_1 = \frac{5}{42}, \quad \lambda_2 = \frac{5}{14}, \quad \lambda_3 = \frac{3}{7}, \quad \lambda_4 = \frac{1}{7}.$$

The resulting method has the same (algebraic) order p as (3.3), but an increased order of dispersion q . Alternatively, we may require that $p = 3$ and $q = 6$. This is achieved by replacing the equation $\beta_4 = 4/105$ by the equation

$$\frac{1}{25}\lambda_1 + \frac{1}{9}\lambda_2 + \frac{1}{4}\lambda_3 + \lambda_4 = \frac{1}{3},$$

to obtain the solution

$$\lambda_0 = -\frac{5}{56}, \quad \lambda_1 = \frac{25}{112}, \quad \lambda_2 = \frac{75}{112}, \quad \lambda_3 = -\frac{1}{14}, \quad \lambda_4 = \frac{15}{56}.$$

Example 3.3. A family of third order methods. It was shown in [9, p. 116] that the method

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

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

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

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

where β_3 should satisfy the relation $\beta_3 = 1/6 + O(h)$ as $h \rightarrow 0$.

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

(3.7)	$\begin{array}{c} 32/85 \\ 8/15 \\ 2/3 \end{array}$	$\begin{array}{c c} 32/85 & 32/85 \\ \hline 1/4 & 17/60 \\ 1/4 & 0 \quad 5/12 \end{array}$	$\begin{array}{l} p=3, \quad q=6, \quad r=3, \\ c=-1/630, \\ (0, \beta) \approx (0, 2.66), \end{array}$
		$\begin{array}{c c} 1/4 & 0 \quad 0 \quad 3/4 \end{array}$	
(3.8)	$\begin{array}{c} 128/429 \\ 256/495 \\ 8/15 \\ 2/3 \end{array}$	$\begin{array}{c c} 128/429 & 128/429 \\ \hline 1/4 & 429/2380 \\ 1/4 & 0 \quad 17/60 \\ 1/4 & 0 \quad 0 \quad 5/12 \end{array}$	$\begin{array}{l} p=3, \quad q=8, \quad r=3, \\ c=-1/28350, \\ (0, \beta) \approx (0, 3.38), \end{array}$
		$\begin{array}{c c} 1/4 & 0 \quad 0 \quad 0 \quad 3/4 \end{array}$	
(3.9)	$\begin{array}{c} 512/1899 \\ 512/1415 \\ 160/357 \\ 8/15 \\ 2/3 \end{array}$	$\begin{array}{c c} 512/1899 & 512/1899 \\ \hline 1/4 & 633/5660 \\ 1/4 & 0 \quad 283/1428 \\ 1/4 & 0 \quad 0 \quad 17/60 \\ 1/4 & 0 \quad 0 \quad 0 \quad 5/12 \end{array}$	$\begin{array}{l} p=3, \quad q=10, \quad r=3, \\ c=-1/2182950, \\ (0, \beta) \approx (0, 3.99). \end{array}$
		$\begin{array}{c c} 1/4 & 0 \quad 0 \quad 0 \quad 0 \quad 3/4 \end{array}$	

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

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

where β_3 and β_4 are defined by

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

here, the z_j are given by (2.15) for $q_0=2$.

It should be observed that, since the zeros z_j depend on h (recall that $\nu := \omega h$, $\bar{\nu} := \bar{\omega} h$), the parameters β_3 and β_4 in (3.10a) will also depend on h ; hence the RK method (3.10) changes if h changes. For small h , it is easily shown that

$$\beta_3 = \frac{1}{6} - \frac{1}{630} z_1^2 z_2^2 + O(h^6), \quad \beta_4 = \frac{1}{30} + \frac{1}{630} (z_1^2 + z_2^2) + O(h^4).$$

Substitution into (2.3) yields

$$\begin{aligned} \phi(\nu) &= \nu^3 \left[\beta_3 - \frac{1}{6} + \left(\beta_4 - \frac{1}{30} \right) \nu^2 + \frac{1}{3} \left(\beta_4 - \frac{4}{105} \right) \right] + O(h^9) \\ &= \frac{\nu^3}{630} [-z_1^2 z_2^2 + \nu^2 (z_1^2 + z_2^2) - \nu^4] + O(h^9), \end{aligned}$$

showing that (3.10) has the same orders $p=2$ and $q=6$ as (3.7) for a fixed interval of frequencies $[\omega, \bar{\omega}]$.

From a practical point of view it is of interest to consider the dispersion ϕ for fixed $(h, \omega, \bar{\omega})$ and varying ω (recall that $(i\omega)^k$ in (1.2) may be interpreted as an eigenvalue of the Jacobian matrix of the ODE to be integrated). Thus, we consider $\phi = \phi(\nu)$ with fixed $\bar{\nu}$ and $\bar{\nu}$. Choosing $\bar{\nu} = 0.5$ and $\bar{\nu} = 1.0$, we find that $\beta_3 \approx .16610021$ and $\beta_4 \approx .03530415$. The corresponding dispersion function $\phi(\nu)$ is plotted in Fig. 3.1.

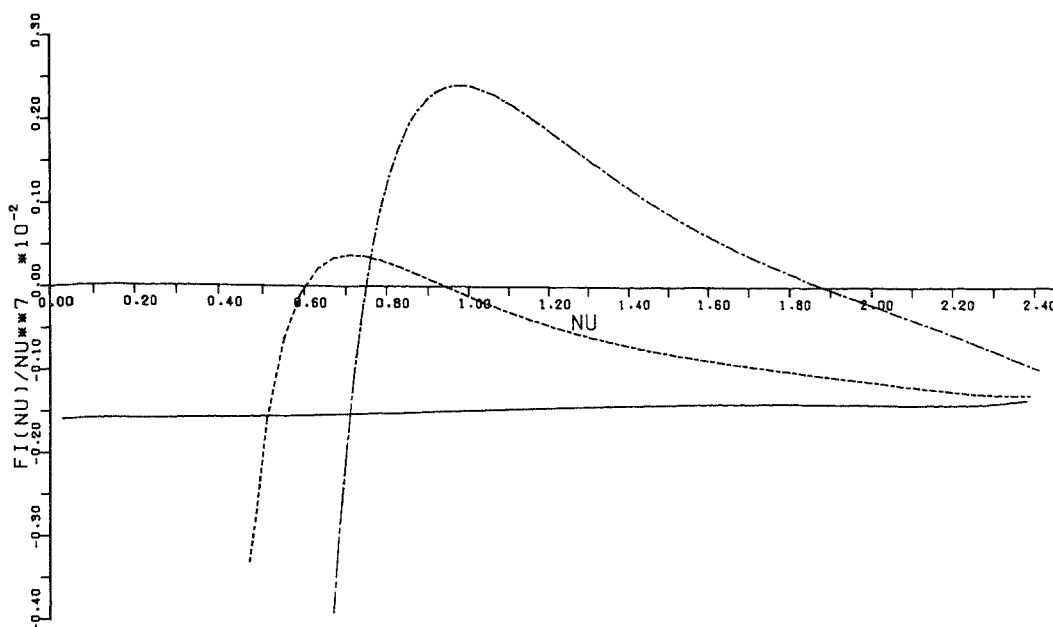


FIG. 3.1. Behaviour of $\phi(\nu)/\nu^7$ for the methods (3.7) (—), (3.10) (---) and Bettis' method (— · —).

In addition, we have plotted the dispersion of (3.7) ($\beta_3 = 1/6, \beta_4 = 1/30$) and of the four-stage method of Bettis with the coefficients chosen to integrate $\nu = 0.75$ exactly, resulting in $\beta_3 \approx .16204146$ and $\beta_4 \approx .04089322$. This picture clearly shows that the “minimax” version (3.10) has a small phase lag if ν lies in the interval $[0.5, 1.0]$. Furthermore, it is obvious that Bettis' method is rather sensitive to a correct estimate of the frequency of the solution. Finally, method (3.7) shows the expected order behavior and its error constant $-1/630$ is easily recognized.

3.2. Runge-Kutta-Nyström methods. The examples constructed below will be represented by the array

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

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 considerations to $m \leq 4, p = 2, 3$ and zero-dissipative methods, that is $P(z) \equiv 1$. Additionally, we constructed several dissipative RKN schemes (i.e. $P(z) < 1$ for $z \in (0, \beta)$). These schemes can be found in the Appendix.

Example 3.4. A family of second order methods with zero-dissipation. Following [10], we consider methods generated by an array of the form

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

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

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

It may be of interest to remark that the family (3.12) turns out to have *zero inhomogeneous dispersion* [13].

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

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

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

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

As a last member of this family, we mention the method

$$(3.16a) \quad \begin{array}{c|ccc} 1/2 & 0 & & \\ 1/2 & 0 & \sigma_3/\sigma_2 & \\ 1/2 & 0 & 0 & \sigma_2 \\ \hline & 0 & 0 & 0 & 1/2 \\ & 0 & 0 & 0 & 1 \end{array}.$$

In this scheme, which is based on the “parent” method (3.14), σ_2 and σ_3 are now determined by the minimax conditions (2.18), viz.

$$(3.16b) \quad \sigma_2 z_j^4 - \sigma_3 z_j^6 = 2 \cos(z_j) - 2 + z_j^2, \quad j = 1, 2,$$

where the z_j are defined in (2.15). In a similar way as done for the RK method (3.10), the method (3.16) can be shown to be of algebraic order $p = 2$ and of dispersion order $q = 6$ as $h \rightarrow 0$ and ω and $\bar{\omega}$ fixed.

Example 3.5. 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:

$$(3.17) \quad \begin{array}{r|lll} .926590210660 & .429284709246 & & \\ .421787206165 & .048227503064 & .040724720578 & \\ \hline & .233566863436 & .107544087262 & .1588890449302 \\ & .127854313973 & .261765691855 & .610379994172 \end{array}$$

where

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

4. Numerical experiments. In this section we show that the methods derived in the preceding section on the basis of the test equation (1.5), may also be superior to conventional methods in nonmodel problems.

4.1. First order equations.

Problem 4.1. Hyperbolic equation:

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

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

$$(4.2) \quad dy/dt = 1/2\Delta x \begin{pmatrix} 0 & -1 & & & \\ 1 & 0 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & & 1 & 0 & -1 \\ & & & -1 & 4 & -3 \end{pmatrix} y.$$

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 20th component of the exact solution vector y reaches its 500th zero at the point

$$(4.3) \quad Z_{500} = 33.509996948 \dots$$

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

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

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

In Table 4.1 the sd-values obtained by the various methods constructed in § 3.1 are listed, together with the results produced by the conventional standard fourth-order method RK4. 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 algebraic order p .

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

4.2. Second order equations.

Problem 4.2. Wave equation:

$$(4.5) \quad \begin{aligned} \frac{\partial^2 u}{\partial t^2} &= gd(x) \frac{\partial^2 u}{\partial x^2} + \frac{1}{4} \lambda^2(x, u)u, \quad 0 \leq x \leq b, \quad t \geq 0, \\ \frac{\partial u}{\partial x}(t, 0) &= \frac{\partial u}{\partial x}(t, b) = 0, \\ u(0, x) &= \sin\left(\frac{\pi x}{b}\right), \quad \frac{\partial u}{\partial t}(0, x) = -\frac{\pi}{b} \sqrt{gd} \cos\left(\frac{\pi x}{b}\right). \end{aligned}$$

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 .

By using second-order symmetric differences, this problem was converted into a system of ODEs and integrated by method (3.13) and, for reasons of comparison, by the second-order Störmer method (see e.g. [16, p. 260]), a well-known explicit scheme for the integration of hyperbolic equations.

For the parameters in problem (4.5) we choose

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

Figure 4.1 shows the results for the ninth component of the system of ODEs (i.e. the one which approximates $u(t, x)$ at $x = 8\Delta x = 80$) in the interval $3567 \leq t \leq 3600$. Scheme (3.13) was applied with $h = 2/3$ and Störmer's method used $h = 1/3$; hence, both methods required the same number of right-hand side evaluations on the whole range of integration. Moreover, we determined a reference solution using scheme (3.14) with $h = 1/30$.

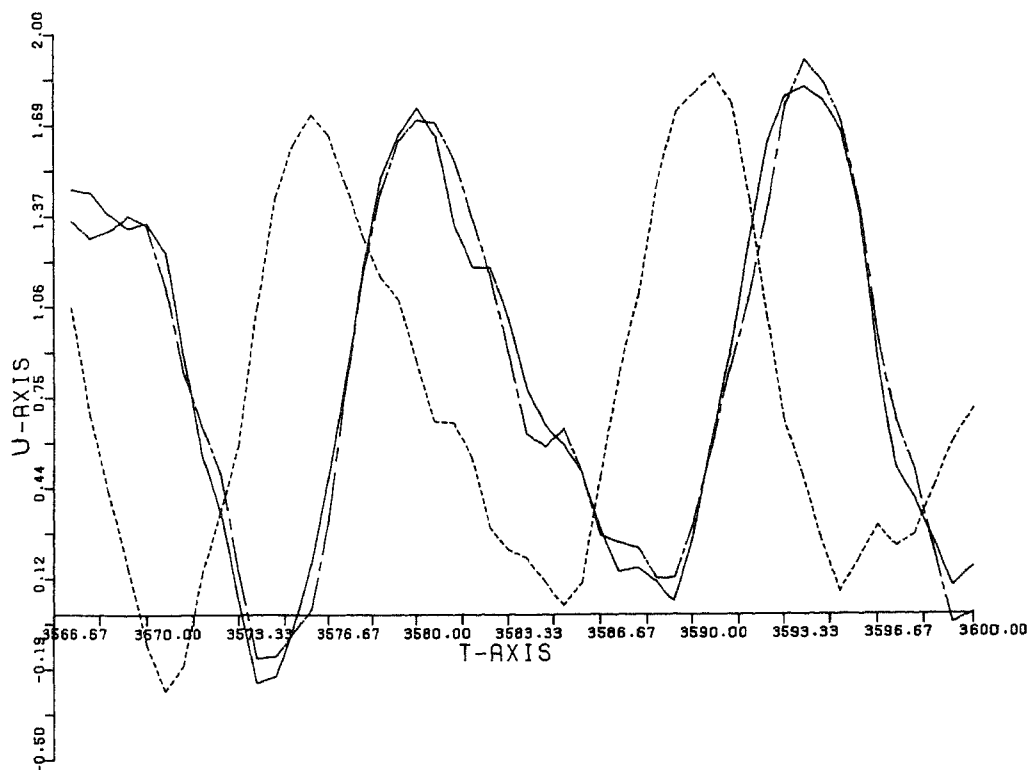


FIG. 4.1. Reference solution (—) of problem (4.5) and the solutions obtained by the Runge-Kutta-Nyström method (3.13) (---) and by the Störmer method (-.-).

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

Problem 4.3. Bessel equation:

$$(4.6) \quad \begin{aligned} \frac{d^2y}{dt^2} &= -\left(100 + \frac{1}{4t^2}\right)y, & t \geq 1, \\ y(t) &= \sqrt{t}J_0(10t). \end{aligned}$$

In order to show that high-order dispersive methods are suitable for long interval integration, we have applied both the conventional fourth-order Nyström method, given by

1/2	1/8		
1	0	1/2	
	1/6	1/3	0
	1/6	2/3	1/6

as well as the methods constructed in § 3.2 on relatively large integration intervals. As before, all experiments required the same computational effort. The accuracy was measured by

$$(4.7) \quad sd(T) := -\log_{10} \left(\max_{n=1, \dots, (T-1)/h} |y(t_n) - y_n| \right)$$

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

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

Method	$[\omega, \bar{\omega}]$	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)	[10, 10.1]	1/20	3	2	6	∞	2	2.9	2.9	2.9	2.9
(3.16)	[9, 11]	1/20	3	2	6	∞	2	2.9	2.9	2.9	2.9
(3.17)	—	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 methods 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 lose accuracy, whereas for method (3.15), having $q = 8$, and for the minimax method (3.16) the accumulation of phase errors is not yet visible on these time-intervals.

Problem 4.4. Inhomogeneous equation:

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

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

We continue 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., ωh not small), because the high-order dispersion will take care of the rapidly oscillating component and the algebraic order, although modest, will take care of the slowly varying component.

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

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 Table 4.3, show the same tendency as was mentioned in the previous example.

Problem 4.5. Orbit equation. Finally, we give an example of a weakly forced oscillation. In [17], Stiefel and Bettis study a slightly perturbed circular orbit in the

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

Method	$[\omega, \bar{\omega}]$	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)	[9.9, 10.1]	1/20	3	2	6	∞	2	1.7	1.7	1.7	1.7
(3.16)	[9, 11]	1/20	3	2	6	∞	2	1.7	1.7	1.7	1.7
(3.17)	—	1/20	3	3	6	∞	3	2.7	2.7	2.4	1.7

TABLE 4.4
sd-values and p_{eff} -values for the orbit equation (4.9).

	Nyström	(3.13)	(3.14)	(3.15)	(3.16) [$\omega, \bar{\omega}$] = [.9, 1.1]	(3.17)
<i>m</i>	3	2	3	4	3	3
<i>p</i>	4	2	2	2	2	3
<i>q</i>	4	4	6	8	6	6
<i>r</i>	5	∞	∞	∞	∞	∞
<i>s</i>	4	2	2	2	2	3
<i>h</i>	$\pi/4$	$\pi/6$	$\pi/4$	$\pi/3$	$\pi/4$	$\pi/4$
$\epsilon = 0$						
<i>sdu(h)</i>	1.1	4.0	6.5	8.7	9.9	5.1
<i>sdu(h/2)</i>	2.7 > 5.3	6.5 > 8.3	10.2 > 12.3	12.6 > 13	12.7 > 9.3	7.9 > 9.3
<i>sdv(h)</i>	0.9	1.9	3.1	4.3	4.8	3.1
<i>sdv(h/2)</i>	2.0 > 3.7	3.1 > 4	4.9 > 6	6.7 > 8	6.6 > 6	4.9 > 6
<i>sdz(h)</i>	0.8	1.9	3.1	4.3	4.8	3.1
<i>sdz(h/2)</i>	2.0 > 4	3.1 > 4	4.9 > 6	6.7 > 8	6.6 > 6	4.9 > 6
$\epsilon = 10^{-6}$						
<i>sdu(h)</i>	1.1	4.0	6.5	8.4	9.2	5.2
<i>sdu(h/2)</i>	2.7 > 5.3	6.4 > 8	9.5 > 10	11.2 > 9.3	11.1 > 6.3	7.2 > 6.7
<i>sdv(h)</i>	0.9	1.9	3.1	4.3	4.9	3.1
<i>sdv(h/2)</i>	2.0 > 3.7	3.1 > 4	4.9 > 6	6.3 > 6.7	6.8 > 6.3	4.9 > 6
<i>sdz(h)</i>	0.8	1.9	3.1	4.3	4.9	3.1
<i>sdz(h/2)</i>	2.0 > 4	3.1 > 4	4.9 > 6	6.3 > 6.7	6.8 > 6.3	4.9 > 6
$\epsilon = 10^{-3}$						
<i>sdu(h)</i>	1.1	3.3	4.6	5.7	6.3	3.3
<i>sdu(h/2)</i>	2.6 > 5	4.6 > 4.3	6.4 > 6	8.2 > 8.3	8.1 > 6	4.1 > 2.7
<i>sdv(h)</i>	0.9	1.9	2.6	2.6	2.8	3.1
<i>sdv(h/2)</i>	2.0 > 3.7	3.2 > 4.3	3.4 > 2.7	3.2 > 2	3.4 > 2	4.9 > 6
<i>sdz(h)</i>	0.8	1.9	2.6	2.6	2.8	3.0
<i>sdz(h/2)</i>	2.0 > 4	3.2 > 4.3	3.4 > 2.7	3.2 > 2	3.4 > 2	4.1 > 3.7

complex plane, described by

$$(4.9) \quad \ddot{z}(t) + z(t) = \varepsilon e^{it}, \quad z \in \mathbb{C}, \quad z(0) = 1, \quad \dot{z}(0) = (1 - \frac{1}{2}\varepsilon)i,$$

whose exact solution is given by

$$(4.10) \quad z(t) = u(t) + iv(t) = [\cos(t) + \frac{1}{2}\varepsilon t \sin(t)] + i[\sin(t) - \frac{1}{2}\varepsilon t \cos(t)].$$

As this example is intended to illustrate the influence of a small inhomogeneous solution component, rather than to show the long term behaviour, we now integrate on a fixed time interval ($0 \leq t \leq 40\pi$) and we list, for a few values of ε , the accuracies of u , v and z , respectively, defined by

$$(4.11) \quad \begin{aligned} sdu(h) &:= -\log_{10} |u_n - u(t_n)|, \\ sdv(h) &:= -\log_{10} |v_n - v(t_n)|, \\ sdz(h) &:= -\log_{10} |z_n - z(t_n)|, \end{aligned}$$

with $t_n = 40\pi$. In Table 4.4 the accuracies obtained are given for two values of h , together with the effective orders of accuracy defined by

$$(4.12) \quad p_{\text{eff}} := \frac{sd(h/2) - sd(h)}{\log_{10}(2)} \approx \frac{sd(h/2) - sd(h)}{.3}.$$

For $\varepsilon = 0$, (4.9) reduces to the model problem so that the analysis should rigorously apply. Since the point $t_n = 40\pi$ is a zero of the component $v(t)$ we expect that sdv presents a reasonable estimate of the phase error of v and should therefore be governed by the homogeneous dispersion orders q and s . In Table 4.4 the sdv values show the order q of propagated dispersion reasonably well; apparently, the initial dispersion does not affect the order of accuracy of v . The accuracy of the u -component is relatively high, so that the total solution $z = u + iv$ exhibits the homogeneous propagated order of dispersion.

For $\varepsilon = 10^{-6}$, (4.9) becomes a slightly perturbed model problem. The results in Table 4.4 show hardly any difference from the case $\varepsilon = 0$. Thus, we conclude that the behaviour of the numerical solution is still mainly determined by the homogeneous components.

For $\varepsilon = 10^{-3}$, Table 4.4 indicates a considerable loss of accuracy for methods (3.14)-(3.17). The inhomogeneous perturbation now introduces a significant inhomogeneous solution component, so that the numerical error does not only consist of errors of homogeneous origin, but also of errors of inhomogeneous origin, i.e., inhomogeneous dispersion and dissipation errors. Therefore, for all methods, except for Nyström's method, a drop in accuracy is to be expected because they are designed to damp *homogeneous errors* in the first place (recall, however, that methods (3.13)-(3.16) which belong to the family (3.12), introduce inhomogeneous dissipation, but no inhomogeneous dispersion).

Finally, we conclude from Table 4.4 that the high-order dispersion methods are superior to the conventional Nyström method irrespective of whether they show their (homogeneous) dispersion order or not.

Appendix.

A1. Additional methods. 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-Kutta-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 σ_j and π_j . The Runge-Kutta-Nyström parameters, expressed in terms of σ_j , are then given by (cf. [10])

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

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 $|\tilde{a}_{\pm}(\nu)| < 1$.

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

$$(A1.2) \quad \begin{array}{c|ccc} .266830712 & 0 & & \\ \hline .065635306 & 0 & -.183849014 & \\ \hline 1/2 & 0 & 0 & 1/12 \\ \hline & 0 & 0 & 0 & 1/2 \\ & 0 & 0 & 0 & 1 \end{array} \quad \begin{array}{l} p=2, \quad q=10, \quad r=3, \\ (0, \beta) \approx (0, 2.40). \end{array}$$

Here,

$$\begin{aligned} \sigma_1 &= 1, & \sigma_2 &= .04713627554, & \sigma_3 &= -.01174842249, \\ \pi_1 &= 0, & \pi_2 &= -.03619705780, & \pi_3 &= .00357232863. \end{aligned}$$

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 § 3.2, 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 Λ 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 β 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:

$$(A1.3) \quad \begin{array}{c|ccc} .4969003529 & .1234549803 & & \\ \hline .7337223214 & .1504173630 & .1187568595 & \\ \hline & .2260389606 & .1450231299 & .1289379095 \\ & .2265821428 & .2849142164 & .4885036408 \end{array}$$

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

$$(A1.4) \quad \begin{array}{ccc|ccc} .4955018983 & & & .1227610656 & & \\ .7166211542 & & & .1493614124 & .1074115269 & \\ \hline & & & .2280103951 & .1277448126 & .1442447923 \\ & & & .2319401058 & .2279673366 & .5400925576 \end{array}$$

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

$$(A1.5) \quad \begin{array}{ccc|ccc} .4940895709 & & & .1220622521 & & \\ .7075002625 & & & .1489112009 & .1013671098 & \\ \hline & & & .2296630303 & .1152557560 & .1550812137 \\ & & & .2348807666 & .1936269363 & .5714922971 \end{array}$$

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 $r = 5$:

$$(A1.6) \quad \begin{array}{ccc|cccc} .0551594317 & & & .0015212815 & & & \\ .6683701446 & & & -1.1732016116 & 1.3965609367 & & \\ .3632109628 & & & 1.5887403855 & -1.7263289145 & .2035496308 & \\ \hline & & & .4046440250 & -.3464696799 & .0829134999 & .3589121550 \\ & & & -1.8067389251 & 2.6410990864 & .9639436971 & -.7983038584 \end{array}$$

Its stability interval is $(0, 3.59)$.

A2. Coefficients of the stability polynomials. As it may be convenient for the reader to have available the coefficients of the stability polynomials in terms of the parameters of the RK(N) method, we give some of these coefficients.

Runge-Kutta methods. The first few parameters β_j as defined in (2.8) are given by

$$(A2.1) \quad \begin{aligned} \beta_2 &= \sum_{j=1}^{m-1} \lambda_{m,j} \sum_{l=0}^{j-1} \lambda_{j,l}, & \beta_3 &= \sum_{j=2}^{m-1} \lambda_{m,j} \sum_{l=1}^{j-1} \lambda_{j,l} \sum_{i=0}^{l-1} \lambda_{l,i}, \\ \beta_4 &= \sum_{j=3}^{m-1} \lambda_{m,j} \sum_{l=2}^{j-1} \lambda_{j,l} \sum_{i=1}^{l-1} \lambda_{l,i} \sum_{k=0}^{i-1} \lambda_{i,k}, \quad \text{etc.} \end{aligned}$$

Runge-Kutta-Nyström methods. The coefficients σ_j and π_j , occurring in the polynomials $S(z)$ and $P(z)$ (cf. (2.11) and (2.14)), can easily be deduced from the coefficients of the polynomials $A_m(z)$, $B_m(z)$, $A_m^*(z)$ and $B_m^*(z)$ (see also (2.7)). We calculated a few terms of these polynomials:

$$(A2.2) \quad \begin{aligned} A_m(z) &= 1 + z \sum_{l=0}^{m-1} \lambda_{m,l} + z^2 \sum_{l=1}^{m-1} \lambda_{m,l} \sum_{k=0}^{l-1} \lambda_{l,k} + \dots, \\ B_m(z) &= 1 + z \sum_{l=1}^{m-1} \lambda_{m,l} \mu_l + z^2 \sum_{l=2}^{m-1} \lambda_{m,l} \sum_{k=1}^{l-1} \lambda_{l,k} \mu_k + \dots, \\ A_m^*(z) &= z \sum_{l=0}^{m-1} \lambda'_l + z^2 \sum_{l=1}^{m-1} \lambda'_l \sum_{k=0}^{l-1} \lambda_{l,k} + \dots, \end{aligned}$$

$$B_m^*(z) = 1 + z \sum_{l=1}^{m-1} \lambda_l' \mu_l + z^2 \sum_{l=2}^{m-1} \lambda_l' \sum_{k=1}^{l-1} \lambda_{l,k} \mu_k + \dots$$

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