HIGH PHASE-LAG ORDER RUNGE-KUTTA AND NŸSTROM PAIRS

S. N. PAPAKOSTAS[†] [‡] AND CH. TSITOURAS[†] [§]

Abstract. We exploit the freedom in the selection of the free parameters of one family of eighth algebraic-order Runge-Kutta pairs and of three families of fourth, sixth, and eighth order (Runge-Kutta)-Nÿstrom pairs with the purpose of obtaining specific pairs of the highest possible phase-lag order, which are also characterized by minimized principal truncation error coefficients. We present a method for the analytic derivation of the dissipation-order conditions for Runge-Kutta methods and the phase-lag and dissipation order conditions for Nÿstrom methods. The Runge-Kutta pairs we study here are based on a one parameter generalization of some older families of pairs. An algorithm and specific optimized 8(6) Nÿstrom pairs are also provided. For a class of initial value problems, whose solution is known to be described by free oscillations or free oscillations of low frequency with forced oscillations of high frequency superimposed, over long integration intervals, these new pairs seem to offer some advantages with respect to some older pairs. The latter are of the same algebraic orders as the new ones, but are characterized by the minimal phase-lag order according to their algebraic-order and number of stages.

Key words. Runge-Kutta, Nÿstrom methods, periodic initial value problems, pairs of embedded methods, hyperbolic equations, phase-lag, dispersion order

AMS subject classification. 65L05

1. Introduction. In a previous work [10] (and its enhanced version [11]) the authors considered the problem of the construction of specially devoted methods for periodic initial value problems of the form

$$y' = f(x, y), \quad y(x_0) = y_0 \qquad x \in [x_0, x_e], \quad f : R \times R^m \to R^m \tag{1.1}$$

whenever f is supposed to be sufficiently smooth and the problem (1.1) is known to be characterized by a solution described by free oscillations or free oscillations of low frequency with forced oscillations of high frequency superimposed, over long integration intervals. Runge-Kutta (RK) methods for problems of this type were introduced by Houwen and Sommeijer in [8].

One method for solving (1.1) numerically, particularly for problems with a low cost in function evaluations, is by means of explicit high order RK pairs. An s-stage RK pair is characterized by a set of coefficients in A, b, $\hat{b}$, c ($A \in R^{s\times s}$, b^T, $\hat{b}^T$, $c \in R^s$), and it is applied on problem (1.1) in the following way. Given the approximate solution $y_n \simeq y(x_n)$ at the point x_n, an approximation $y_{n+1} \simeq y(x_{n+1})$ is computed at x_{n+1} from the formulas

$$y_{n+1} = y_n + h_n \sum_{i=1}^{s} b_i k_i,$$

where $h_n = x_{n+1} - x_n$,

$$k_1 = f(x_n, y_n),$$

[†] National Technical University of Athens, Department of Mathematics, Zografou Campus, Athens 157 80, GREECE.

[‡] (spapakos@@softlab.ece.ntua.gr)

[§] (tsitoura@@math.ntua.gr)

$$k_j = f\left(x_n + h_n c_j, y_n + h_n \sum_{i=1}^{s-1} a_{ji} k_i\right), \quad j = 2, 3, \ldots, s,$$

and the error quantity

$$e_{n+1} = h_n \sum_{i=1}^{s} \left(b_i - \hat{b}_i\right) k_i$$

is used for the purposes of step-size control (see Shampine [16]).

A RK pair is said to be of an algebraic order $p(q)$ $(p > q)$, whenever both its associated RK methods (characterized by A, b, c and A, $\hat{b}$, c respectively) satisfy a set of polynomial order conditions, being in one-to-one correspondence with the set of (rooted) trees T (see for example Hairer, Nörsett and Wanner [7], or Butcher [1]). The solution of this system of order conditions is usually carried out through the use of various types of simplifying assumptions (the most commonly used are those of the type discussed by Curtis [2], Butcher [1] and theoretically justified in [12]). All known RK methods and pairs of orders exceeding four satisfy the simplifying assumption $Ae = c$, $e = \underbrace{\{1, \ldots, 1\}}_{s}^{T}$.

The application of a RK method to the test problem

$$y' = i\omega y, \quad \omega \in R \tag{1.2}$$

leads to the numerical scheme $y_{n+1} = P(\omega h_n) y_n$, $h_n = x_{n+1} - x_n$, where the function $P(v) = P(\omega h)$ satisfies the relation $P(v) = 1 + vb(I - vA)^{-1} e = \sum_{i=0}^{\infty} t_i v^i$, and for $i \geq 1$, $t_i = bA^{i-1}e$, $t_0 = 1$. The numbers t_i depend only on the coefficients of the method. It must be observed that for explicit methods (that is for A lower triangular), the summation in the determination of $P(v)$ above is finite (specifically, i runs from 0 through s).

The phase-lag (or dispersion) order of a RK method is defined as the order of approximation of the argument of the exponential function by the argument of P along the imaginary axis. Symbolically, the phase-lag order of a method is q, whenever $\delta(v) = O\left(v^{q+1}\right)$, for $\delta(v) = v - \arg(P(v))$. For RK methods this notion has been introduced in [8]. The imaginary stability interval of a RK method $I_I = (0, v_0)$ is defined by the relations $|P(v)| < 1$ and $|P(v_0 + \theta)| > 1$, for every $v \in I_I$ and every suitably small positive θ. A method characterized by a non-vanishing imaginary stability interval is called dissipative.

Although for a RK method the phase-lag property is defined for the special problem (1.2), as it was shown by the numerical tests presented in [10], RK pairs of high phase-lag order exhibit a remarkable numerical performance on a much wider class of test problems. It seems that for a certain class of initial value problems (as those whose solutions are described by free oscillations or free oscillations of low frequency with forced oscillations of high frequency superimposed, over long integration intervals), it might be advantageous to use pairs of methods of high phase-lag order with minimized their leading truncation error coefficients instead of pairs of the same algebraic order as the latter, but with a phase-lag order equal to the minimal allowed by the number of stages and their algebraic order.

In this article we intend to further explore these assertions by obtaining high algebraic-order, high phase-lag order RK pairs. We also intend to study the numerical performance of (Runge-Kutta)-Nÿstrom (RKN) pairs applied on a special second-order initial value problem of the form

$$
\begin{array}{l}
y'' = f(x, y), \quad y(x_0) = y_0, \quad y'(x_0) = y'_0 \\
x \in [x_0, x_e], \quad f : R \times R^m \to R^m
\end{array}
\tag{1.3}
$$

which is known to be characterized by a periodic solution. Nÿstrom pairs are characterized by the coefficients in A, b, b', $\hat{b}$, $\hat{b}'$, and c, where $A \in R^{s\times s}$ and b^T, b'^T, $\hat{b}^T$, $\hat{b'}^T$, $c \in R^s$. If $y_n \simeq y(x_n)$, $y'_n \simeq y'(x_n)$ is the solution, and its derivative, computed at the point x_n, then these pairs are applied on (1.3) in order to approximate $y_{n+1} \simeq y(x_{n+1})$, $y'_{n+1} \simeq y'(x_{n+1})$ at x_{n+1} according to the formulas

$$
\begin{aligned}
y_{n+1} &= y_n + h_n y'_n + h_n^2 \sum_{i=1}^{s} b_i k_i, \\
y'_{n+1} &= y'_n + h_n \sum_{i=1}^{s} b'_i k_i,
\end{aligned}
$$

where

$$
\begin{aligned}
k_1 &= f(x_n, y_n), \\
k_j &= f\left(x_n + h_n c_j, y_n + h_n y'_n + h_n^2 \sum_{i=1}^{s-1} a_{ji} k_i\right), \quad j = 2, 3, \ldots, s,
\end{aligned}
$$

and some norm of the vector $\left(e_{n+1}^T, \left(e'_{n+1}\right)^T\right)^T$, with

$$
\begin{aligned}
e_{n+1} &= h_n^2 \sum_{i=1}^{s} \left(b_i - \hat{b}_i\right) k_i, \\
e'_{n+1} &= h_n \sum_{i=1}^{s} \left(b'_i - \hat{b}'_i\right) k_i,
\end{aligned}
$$

is used for feeding the step-size change control algorithm.

For higher order pairs it is advantageous to consider the following set of simplifying assumptions

$$
\begin{aligned}
Ae &= \frac{c^2}{2} \\
b &= b'(I - C) \\
\hat{b} &= \hat{b}'(I - C)
\end{aligned}
$$

where $C = \operatorname{diag}(c)$. None of these conditions is absolutely necessary (see for example the low algebraic order methods of Houwen and Sommeijer [8]), but their application, especially for higher order methods and pairs, greatly simplifies the system of non-linear order conditions.

In the next section we shall seek explicit formulas for the determination of the phase-lag and dissipation order of RK and Nÿstrom methods. In the third section we shall describe the derivation of special eighth algebraic-order RK pairs, which belong to a three-parameter (b_{13}, $\hat{b}_{12}$, and $\hat{b}_{13}$) extension of the family proposed by

Verner in [18] and studied theoretically in its full generality, leading to the only known efficiently implementable algorithms in [12]. The type of simplifying assumptions used for the derivation in [18] (as well as in other newer ones) are based on those proposed by Fehlberg [6]. In particular, the implied derivation by Prince and Dormand [15] (which does not contain any algorithms) seems to miss the free parameter $\hat{b}_{13}$. High phase-lag order Nÿstrom pairs of algebraic orders 4(3), 6(4), and 8(6) are derived in the fourth section. As we have found in practice (see also [10]), for the types of periodic initial value problems studied here, it seems to be more advantageous to consider pairs of the highest achievable phase-lag order, instead of pairs of high dissipative order as well. In the last section we evaluate the numerical performance of all new RK and Nÿstrom pairs proposed by our study, with respect to other existing pairs of the same algebraic orders, which however were not specifically designed for periodic initial value problems.

2. Phase-Lag and dissipation order of Runge-Kutta and Nÿstrom methods. The dissipation order of a RK method (see Houwen and Sommeijer [8]) is defined as the order of approximation of the modulus of the exponential function by the modulus of the characteristic function $P(v)$ of the method along the imaginary axis. That is the dissipation order is q, *iff* $\alpha(v) = O(v^{q+1})$, for $\alpha(v) = 1 - |P(v)|$. In practical situations one is interested in estimating both the phase-lag and dissipation order of a pth algebraic-order RK method. Let $t_i = bA^{i-1}e$ and $t_{-1} = 0$. Explicit formulas for both these quantities are offered by the following theorem.

THEOREM 2.1 (PHASE-LAG AND DISSIPATION ORDER CONDITIONS FOR RK METHODS). *A RK method is of phase-lag order* $2r_p$ iff *for every* $k = 1, \ldots, r_p$,

$$X_p(k) = 0 \text{ and } X_p(r_p+1) \neq 0,$$

where

$$X_p(k) = \sum_{n=1}^{k} \frac{2^{2(k-n+1)}\left(2^{2(k-n+1)}-1\right)}{(2(k-n+1))!} B_{2(k-n+1)} t_{2n-2} - t_{2k-1},$$

and $B_{2n} = B_{2n}(0)$ *are the Bernoulli numbers.*

Moreover a method is of dissipation order $r_d \geq 2$ iff *for every* $k = 2, \ldots, r_d$, $\tilde{X}_d(k) = 0$ *and* $\tilde{X}_d(r_d+1) \neq 0$, *where*

$$\tilde{X}_d(k) = \sum_{n=1}^{k} \left(t_{2n-2}t_{2(k-n)} + t_{2n-1}t_{2(k-n)-1}\right).$$

Proof. The proof concerning the phase-lag order conditions has been given in [10]. For the dissipation order conditions one should consider the formal expansion

$$\begin{aligned} |P(v)|^2 - 1 &= \left(\sum_{i=1}^{\infty} (-1)^{i+1} t_{2i-2} v^{2i-2}\right)^2 + \left(\sum_{i=1}^{\infty} (-1)^{i+1} t_{2i-1} v^{2i-1}\right)^2 - 1 \\ &= \sum_{i=2}^{\infty} \left(\sum_{j=1}^{i} \left(t_{2j-2}t_{2(i-j)} + t_{2j-1}t_{2(i-j)-1}\right)\right) v^{2i-2}. \end{aligned}$$

□

If a specific method is of algebraic-order p, then one should take into account in the previous theorem, that from the algebraic order conditions it is $t_i = \frac{1}{i!}$, for $0 \leq i \leq p$.

Next consider the test problem

$$y'' = -\lambda^2 y, \quad y(0) = 1, \quad y'(0) = i\lambda, \quad \lambda \in R \tag{2.1}$$

whose exact solution is

$$\bar{y} = e^{i\lambda x} \tag{2.2}$$

When (2.1) is solved numerically by a Nÿstrom method, the following recursive relation is obtained

$$Y_{n+1} = R(z_n) Y_n, \quad z_n = -H_n^2, \quad H_n = \lambda h_n,$$

where $Y_n = [y_n, h_n y_n']^T$ and

$$R(z) = \begin{vmatrix} 1 + zb(I - zA)^{-1} e & 1 + zb(I - zA)^{-1} c \\ zb'(I - zA)^{-1} e & 1 + zb'(I - zA)^{-1} c \end{vmatrix}.$$

The theoretical solution $\bar{Y}_n = \bar{Y}(x_n) = [\bar{y}(x_n), h_n \bar{y}'(x_n)]^T$ of (2.2) satisfies the recursive relation

$$\bar{Y}_{n+1} = \bar{R}(H_n) \bar{Y}_n,$$

where

$$\bar{R}(H_n) = \begin{vmatrix} \cos H_n & \frac{\sin H_n}{H_n} \\ -H_n \sin H_n & \cos H_n \end{vmatrix}.$$

The phase-lag (or dispersion) order of a Nÿstrom method (see [8]) is defined as the order of approximation of the arguments of the eigenvalues of $\bar{R}$ by the argument of the eigenvalues of R. Clearly this is expressed by the number q, where $\tilde{\delta}(v) = O\left(v^{q+1}\right)$ and $\tilde{\delta}(v) = v - \arccos\left(\text{trace}\left(R(z) / \left(2\sqrt{\det R(z)}\right)\right)\right)$.

Let, for $i \geq 1$, $\sigma_{2i-1} = bA^{i-1}e$, $\sigma_{2i} = bA^{i-1}c$, $\sigma'_{2i-1} = b'A^{i-1}e$, $\sigma'_{2i} = b'A^{i-1}c$ and $\sigma'_{-1} = 0$, $\sigma_0 = \sigma_{-1} = \sigma'_0 = 1$. Applying the *formal* Neumann expansion of $(I - zA)^{-1}$ (see Ortega [9], page 201, relation 5.3.18) we may formally write

$$R(z) = \begin{vmatrix} 1 + \sigma_1 z + \sigma_3 z^2 + \cdots & 1 + \sigma_2 z + \sigma_4 z^2 + \cdots \\ \sigma'_1 z + \sigma'_3 z^2 + \cdots & 1 + \sigma'_2 z + \sigma'_4 z^2 + \cdots \end{vmatrix} = \begin{vmatrix} \sum_{i=0}^{\infty} \sigma_{2i-1} z^i & \sum_{i=0}^{\infty} \sigma_{2i} z^i \\ \sum_{i=0}^{\infty} \sigma'_{2i-1} z^i & \sum_{i=0}^{\infty} \sigma'_{2i} z^i \end{vmatrix}.$$

The interval of periodicity of a Nÿstrom method $I_P = (0, v_0)$, applied on problem (2.1), is defined to satisfy $\det(R(z)) \equiv 1$ and $|\text{trace}(R(z))| \leq 2$, for every $z \in I_P$ and $|\text{trace}(R(z + \theta))| > 2$, for some suitable small θ. Methods with an extended interval of periodicity might be especially suited for mildly stiff, oscillatory problems.

THEOREM 2.2 (PHASE-LAG ORDER CONDITIONS FOR NYSTROM METHODS). *A Nÿstrom method is of phase-lag order* $2r_{Np}$ iff *for any* $k = 1, \ldots, r_{Np}$,

$$X(k) = 0 \text{ and } X(r_{Np} + 1) \neq 0,$$

where

$$X_{Np}\,(k) = 2\pi_k - \rho_k + \sum_{n=0}^{k} \frac{2^{2n+1}}{(2n)!} \pi_{k-n},$$

and

$$\begin{aligned} \pi_k &= \sum_{j=0}^{k} \left(\sigma_{2k-2j-1}\sigma'_{2j} - \sigma'_{2k-2j-1}\sigma_{2j} \right), \\ \rho_k &= \sum_{j=0}^{k} \left(\sigma_{2k-2j-1} + \sigma'_{2k-2j} \right) \left(\sigma_{2j-1} + \sigma'_{2j} \right). \end{aligned}$$

Proof. Let $T_p = \mathrm{tr}\,(R)$ and $D_p = \det\,(R)$. We may write

$$T_p = \sum_{i=0}^{\infty} \left(\sigma_{2i-1} + \sigma_{2i} \right) z^i, \tag{2.3}$$

and after performing the multiplications

$$D_p = \sum_{i=0}^{\infty} \left(\sum_{j=0}^{i} \sigma_{2i-2j-1}\sigma_{2j}\prime \right) z^i - \sum_{i=1}^{\infty} \left(\sum_{j=0}^{i-1} \sigma'_{2i-2j-1}\sigma_{2j} \right) z^i.$$

Since $\sigma'_{-1} = 0$, we find

$$D_p = \sum_{i=0}^{\infty} \pi_i z^i. \tag{2.4}$$

After carrying out the necessary multiplication, we may estimate from (2.3)

$$T_p^2 = \sum_{i=0}^{\infty} \rho_i z^i. \tag{2.5}$$

Substituting (2.4), (2.5) in the relation $4D_p \cos^2(z) - T_p^2$ and expanding $\cos^2(z) = \frac{1}{2}\left(1 + \sum_{i=0}^{\infty} \frac{2^{2i}}{(2i)!} z^i\right)$ we find

$$4D_p \cos^2(z) - T_p^2 = 2\sum_{i=0}^{\infty} \pi_i z^i + \left(\sum_{i=0}^{\infty} 2\pi_i z^i \right) \left(\sum_{i=0}^{\infty} \frac{2^{2i}}{(2i)!} z^i \right) - \sum_{i=0}^{\infty} \rho_i z^i,$$

from which we may estimate the required equations as the multipliers in the series

$$4D_p \cos^2(z) - T_p^2 = \sum_{i=0}^{\infty} \left(2\pi_i - \rho_i + \sum_{j=0}^{i} \frac{2^{2j+1}}{(2j)!} \pi_{i-j} \right) z^i.$$

□

3. Some high phase-lag order RK pairs. The solution of the order conditions for the construction of high algebraic-order RK pairs is achieved by means of employing a set of simplifying assumptions. According to the number and type of simplifying assumptions they satisfy, RK pairs belong to certain families of solution of the algebraic-order conditions, characterized by a set of free parameters.

In the following we shall restrict our attention to the family of type Ia (as characterized in [12]), of algebraic order 8(7) with 13 stages. A theoretical study of this family, as well as details of specific algorithms, which may be used for the construction of specific pairs is given in [12]. These pairs are characterized by the condition $a_{13,12} = 0$. Consequently $t_{13} = 0$. According to Theorem 2.1, this restricts the maximal phase-lag order to 16. The phase-lag order conditions in this case result to the following set of additional conditions

$$t_9 = \frac{1}{9!}, \quad t_{10} = \frac{71}{259459200}, \quad t_{11} = \frac{1}{43243200}, \quad t_{12} = \frac{1}{778377600}. \tag{3.1}$$

An alternative approach is to try to increase the phase-lag order of the seventh algebraic-order formula as well. We do not however support this strategy, because many numerical tests we have performed indicate that in general it is more advantageous to use, the otherwise restricted parameters of the family, in order to further minimize the principal truncation error coefficients of the pth-order method of the pair. The free parameters of the 8(7) family of RK pairs are c_2, c_5, c_6, c_7, c_8, c_{10}, c_{11}, a_{87}, b_{13}, $\hat{b}_{12}$, and $\hat{b}_{13}$ (one more parameter than those identified in [15] and three more than those initially proposed in [18]). Since $t_9 = \frac{1}{9!}$, we see that by default these pairs are of a 10th dissipation order.

For the solution of (3.1), along with the algorithms mentioned before, we used both a symbolic algebra manipulation package and its FORTRAN version in conjunction to a numerical minimization routine to find those values of the free parameters, which lead to a minimized value of $\left\|T^{(9)}\right\|_2$. This may be achieved by making use of the *only* widely available (fast) algorithm for this case, based on the theoretical justification proposed in [12]. For incorporating the phase-lag order conditions we proceeded as follows. From (3.1), using a symbolic algebra manipulation package, we express the values of c_5, c_6, c_7, and a_{87} in terms of the remaining free parameters, leaving as free parameters only c_2, c_8, c_{10}, c_{11}, b_{13}, $\hat{b}_{12}$, and $\hat{b}_{13}$. An optimal pair, of phase-lag order 16, (NEW8(7)P) we found to be described by the values of the free parameters

$$\begin{array}{llll} c_2 = \frac{1}{39}, & c_5 = \frac{514748023}{1400737386}, & c_6 = \frac{753846329}{1732179602}, & \\ c_7 = \frac{81892839}{604421644}, & c_8 = \frac{2}{7}, & c_{10} = \frac{10}{13}, & c_{11} = \frac{6}{7}, \\ a_{87} = \frac{551682764}{839617083}, & b_{13} = \frac{1}{18}, & \hat{b}_{12} = -\frac{11}{18}, & \hat{b}_{13} = \frac{11}{18}. \end{array} \tag{3.2}$$

The parameters of this family are presented in Table 3.1. All its major characteristics may be found in Table 3.2. The extended real stability interval was a coincidental side effect of the minimization.

4. High phase-lag order Nÿstrom pairs. We shall first investigate the possibility of constructing high phase-lag order Nÿstrom pairs for the families of algebraic-orders 4(3) and 6(4) suggested and studied by Dormand, El-Mikkawy, and Prince [3], because these seem to be fairly general families of pairs based on a reasonably small number of simplifying assumptions. According to our numerical tests we decided to sacrifice the possibility of obtaining pairs with a non-vanishing interval of periodicity,

TABLE 3.1
Coefficients of NEW8(7)P, selection (10) (rational approximations accurate to 21 significant digits).

0													
$\frac{1}{39}$	$\frac{1}{39}$												
$\frac{1551985603}{15106987586}$	$-\frac{819919454}{7954880963}$	$\frac{1550002331}{7531441519}$											
$\frac{4655956809}{30213975172}$	$\frac{166589347}{4324203682}$	0	$\frac{2244683731}{19421949501}$										
$\frac{514748023}{1400737386}$	$\frac{1434700181}{4526297859}$	0	$\frac{-17244495369}{14827907888}$	$\frac{14672042545}{12090788322}$									
$\frac{753846329}{1732179602}$	$\frac{216865477}{4503783464}$	0	0	$\frac{2363387954}{10609390473}$	$\frac{3736705947}{22745211070}$								
$\frac{81892839}{604421644}$	$\frac{764510756}{13040330925}$	0	0	$\frac{452445933}{4716444208}$	$-\frac{895931653}{22522139750}$	$\frac{873774614}{42183754199}$							
$\frac{2}{7}$	$\frac{199659293}{12702785561}$	0	0	$-\frac{7555597260}{16483583449}$	$\frac{657452440}{5173579471}$	$-\frac{1119897545}{20078489442}$	$\frac{551682764}{839617083}$						
$\frac{6192277787}{12208988746}$	$\frac{793314604}{13976557807}$	0	0	$\frac{2985235807}{7278171282}$	$\frac{14028594}{1101021281}$	$\frac{958376589}{5714262451}$	$-\frac{1974918656}{10673172099}$	$\frac{405612119}{9044847963}$					
$\frac{10}{13}$	$\frac{1266074123}{6281065917}$	0	0	$-\frac{4581355363}{3046479129}$	$-\frac{2937544370}{5006731581}$	$-\frac{2357986081}{765762355}$	$\frac{5335414531}{10119211873}$	$\frac{25789073016}{9056069051}$	$\frac{19094602291}{8082377928}$				
$\frac{6}{7}$	$-\frac{3403758010}{22022585129}$	0	0	$\frac{4666993327}{14783147739}$	$\frac{5262730239}{11622135734}$	$\frac{22432995201}{7608186638}$	$\frac{9127994833}{10060356632}$	$-\frac{33791676863}{14898822572}$	$-\frac{22523121910}{13774108167}$	$\frac{7536718113}{25936600354}$			
1	$-\frac{657508583}{7361604142}$	0	0	$\frac{49525568891}{22957107026}$	$\frac{1115105471}{6543055469}$	$\frac{62486325091}{20061313835}$	$-\frac{6187148133}{7800444566}$	$-\frac{9226813649}{3827536113}$	$-\frac{5946035525}{3942473888}$	$-\frac{387575575}{11448823629}$	$\frac{967235657}{2463131197}$		
1	$\frac{5170243423}{15755825726}$	0	0	$\frac{5017941652}{6447774631}$	$-\frac{1751809551}{4639249355}$	$-\frac{125019663783}{25359617453}$	$-\frac{12406223420}{6830353731}$	$\frac{77341300113}{24385589366}$	$\frac{37789086389}{9899353391}$	$-\frac{5956267453}{11979576404}$	$\frac{2693279968}{5123250599}$	0	
b	$\frac{169842013}{3932943796}$	0	0	0	0	$-\frac{538046068}{6364136977}$	$\frac{3845693529}{21142204130}$	$\frac{1806141113}{11369404446}$	$\frac{1227998211}{3278129960}$	$\frac{701266701}{6738259450}$	$\frac{1126082023}{6379136305}$	$-\frac{51833701}{5104603713}$	$\frac{1}{18}$
$\hat{b}$	$\frac{522276081}{5878413005}$	0	0	0	0	$-\frac{10426657685}{4368315947}$	$-\frac{1159962323}{11041458463}$	$\frac{4105332252}{3814764721}$	$\frac{19903609720}{8774029877}$	$-\frac{7363979475}{14423836544}$	$\frac{5002757021}{8792250993}$	$-\frac{11}{18}$	$\frac{11}{18}$

TABLE 3.2
The main characteristics of the RK and Nystrom pairs compared here.

Type	Pairs of alg. orders $p(q)$	Phase-Lag order	Effective Number of Stages	$\left\|T^{(p+1)}\right\|_2$	$\left\|T'^{(p+1)}\right\|_2$	I_R	I_{IM}	D_∞
RK	NEW8(7)P	16	13	$5.83 \cdot 10^{-6}$		$(-6.55, 0)$	$(0, 0)$	4.9
	PD8(7)	8	13	$4.51 \cdot 10^{-6}$		$(-5.16, 0)$	$(1.51, 3.70)$	16.7
RKN	NEW4(3)P	8	3	$1.1 \cdot 10^{-2}$	$7.4 \cdot 10^{-3}$	$(0, 0)$	$*$	1.5
	DEP4(3)	4	3	$4.6 \cdot 10^{-4}$	$1.8 \cdot 10^{-3}$	$(0, 0)$	$*$	6.1
	NEW6(4)P	10	5	$8.4 \cdot 10^{-5}$	$6.7 \cdot 10^{-5}$	$(0, 5.61)$	$*$	0.69
	DEP6(4)	6	5	$8.7 \cdot 10^{-5}$	$7.7 \cdot 10^{-5}$	$(0, 0)$	$*$	1.1
	NEW8(6)	8	8	$9.9 \cdot 10^{-8}$	$9.4 \cdot 10^{-8}$	$(0, 6.86)$	$*$	27.1
	NEW8(6)P	14	8	$8 \cdot 10^{-7}$	$8.2 \cdot 10^{-7}$	$(0, 0)$	$*$	1.5
	DEP8(6)	8	8	$8.3 \cdot 10^{-7}$	$8.2 \cdot 10^{-7}$	$(0, 3.29)$	$*$	9.7

I_{IM}: Imaginary Stability Interval (not applicable to Nÿstrom methods).
I_R: Real Stability Interval (for Nÿstrom methods this is simply the Stability Interval).
$\left\|T^{(p+1)}\right\|_2$: Euclidean norm of the vector consisting of all the principal truncation error coefficients of the higher order method of a pair (regarding the solution y).
$\left\|T'^{(p+1)}\right\|_2$: as before but regarding $y\prime$,
D_∞: the maximum modulus of all coefficients of a pair.

in favor of finding pairs with maximal phase-lag orders. All the pairs below satisfy the FSAL (First Step As Last) device.

These 4(3) pairs are characterized by the free parameters c_2, c_3, $\hat{b}_3$, $\hat{b}_4$, and $\hat{b}'_4$, of which only $\hat{b}_3$, $\hat{b}_4$, and $\hat{b}'_4$ remain free after imposing the two phase-lag order conditions for order 8 resulting from Theorem 2.2. However the value of $\left\|T^{(5)}\right\|_2$ does not depend on the latter parameters (which for this reason were selected as in DEP4(3)). The coefficients of one of the two uniquely defined pairs (namely that corresponding to the minimal value of $\left\|T^{(5)}\right\|_2$) may be found in Table 4.1.

Similarly, in Table 4.2 may be found a 6(4) pair with minimized truncation error coefficients of phase lag order 10. In this case from the free parameters c_2, c_3, c_4, $\hat{b}'_5$, and $b'_6 = \hat{b}'_6$, only c_4, $\hat{b}'_5$, and b'_6 remain free after imposing the phase-lag order conditions. By inspecting the principal characteristics of this new pair from Table 3.2, we see that NEW6(4)P is comparable to DEP6(4) as a general purpose pair as well.

For the 8(6) pairs we applied the simplifying assumptions used in [4] and we developed the algorithm described in the appendix. The following theorem may be proved along the lines of Proposition 1 and Lemma 1 of [13] and Propositions 1, 2 of [14] concerning RK methods.

THEOREM 4.1. *The coefficients of any Nÿstrom pair derived by applying the algorithm in the appendix characterize a pair of algebraic orders* 8(6).

We should note that although no algorithms or hints of a possible solution were presented in [4], the pair DEP8(6) of [4] is now seen to belong in this exactly new family. Moreover, the derivation implied in [4] seems to be characterized by one parameter less (namely a_{82}). It is known (see [14]; and for another yet justification [13]) that among families of pairs of the same orders (and most notably among those satisfying the same type of simplifying assumptions) it is most probable that the best pairs can be found among those belonging to the family with the larger number of free parameters. The new pairs presented here further support this claim.

First by using a minimization routine we derived the optimized general purpose pair NEW8(6) (see Table 4.3). For finding a 14th phase-lag order, 8(6) algebraic-

TABLE 4.1
Coefficients of NEW4(3)P (rational approximations accurate to 20 digits).

0				
$\frac{5280320246}{8739982487}$	$\frac{379540831}{2079644486}$			
$\frac{2488284716}{4549257065}$	$\frac{4090178078}{30784316359}$	$\frac{724764885}{43347833381}$		
1	$\frac{1382866212}{8058611935}$	$-\frac{958895179}{4232828403}$	$\frac{3246882200}{5850906049}$	
b	$\frac{1382866212}{8058611935}$	$-\frac{958895179}{4232828403}$	$\frac{3246882200}{5850906049}$	0
b'	$\frac{1382866212}{8058611935}$	$-\frac{5103277582}{8917268805}$	$\frac{12283001905}{10027502947}$	$\frac{2640160123}{15021458620}$
$\hat{b}$	$\frac{2788682442}{15739802773}$	$\frac{1966645306}{8825920383}$	$\frac{3}{20}$	$-\frac{1}{20}$
$\hat{b}'$	$\frac{1153046258}{2574473725}$	$\frac{27711564209}{4540932828}$	$-\frac{31509757256}{6039640179}$	$-\frac{1}{3}$

TABLE 4.2
Coefficients of NEW6(4)P (rational approximations accurate to 20 digits).

0						
$\frac{76064096}{555208869}$	$\frac{148104835}{15781657211}$					
$\frac{61651457}{172436989}$	$\frac{83570507}{15621004272}$	$\frac{1008730685}{17224387836}$				
$\frac{473}{677}$	$\frac{313507335}{5002407628}$	$\frac{232561219}{6632504445}$	$\frac{2487592367}{16999280447}$			
$\frac{1521284172}{2494038851}$	$\frac{497059253}{7416116119}$	$-\frac{31814195}{4301239521}$	$\frac{666859859}{4681708182}$	$-\frac{164695106}{10269973361}$		
1	$\frac{1104491309}{17344385380}$	$\frac{2297852298}{21296988487}$	$\frac{1270882233}{4862169760}$	$\frac{1745513301}{8827769149}$	$-\frac{854905921}{6541617807}$	
b	$\frac{1104491309}{17344385380}$	$\frac{2297852298}{21296988487}$	$\frac{1270882233}{4862169760}$	$\frac{1745513301}{8827769149}$	$-\frac{854905921}{6541617807}$	
b'	$\frac{1104491309}{17344385380}$	$\frac{928753894}{7428602053}$	$\frac{1088487657}{2675475233}$	$\frac{2281030107}{3476164510}$	$-\frac{5717085047}{17062458528}$	$\frac{1}{12}$
$\hat{b}$	$\frac{390850314}{4665518297}$	$\frac{879866760}{14012015573}$	$\frac{1237986347}{4111942715}$	$\frac{1838896521}{8824986790}$	$-\frac{1945509358}{12470194255}$	
$\hat{b}'$	$\frac{390850314}{4665518297}$	$\frac{831255784}{11424277409}$	$\frac{5386054494}{11493559817}$	$\frac{5380034471}{7780066871}$	$-\frac{2}{5}$	$\frac{1}{12}$

order pair, with the minimum value of $\left\|T^{(9)}\right\|_2$, we proceeded as follows. Let $l_i = s_i$, $i = 1, 2, 3$ be the general form of each one of the order conditions for a 14th phase-lag order pair. First we employed the explicit general purpose algorithm of the appendix for deriving 8(6) pairs, as a FORTRAN subroutine, and we minimized with respect to $\left\|T^{(9)}\right\|_2$, as well as for the quantities $|l_i - s_i|$, for $i = 1, 2, 3$. Special care was applied so that the minimization of the latter quantities was very close to that allowed by the machine zero. We thus derived at a preliminary estimation of the values of c_4, c_5 which were subsequently truncated (for easing the presentation) at their rational approximations 3/10 and 5/9 respectively. Next we used a symbolic algebra manipulation package (with the values of c_4, c_5 this time fixed) and solved the three phase-lag order conditions with respect to the 45-digit accurate approximations of c_6, c_7, and a_{82}. The coefficients of the pair NEW8(6)P, which was obtained by this procedure, may be found in Table 4.4.

5. Numerical results. We compared NEW8(7) with respect to PD8(7) ([15]) on the same set of test problems as in [10], namely G1, G2, G3, G4, and G5, under Error-Per-Step control and for tolerances 10^{-3}, 10^{-4},..., 10^{-9}. The Nÿstrom pairs were applied on problems G2, G4, G5, but this time we used in place of G1 the

TABLE 4.3
Coefficients of NEW8(6) (rational approximations accurate to 20 digits).

0									
$\frac{531055007}{9538622078}$	$\frac{36116545}{23303892186}$								
$\frac{531055007}{4769311039}$	$\frac{39482639}{19106876692}$	$\frac{39482639}{9553438346}$							
$\frac{307}{910}$	$\frac{693118601}{11824108190}$	$-\frac{397651513}{3359436123}$	$\frac{2504695913}{21470747966}$						
$\frac{311}{517}$	$-\frac{4619407667}{10805040220}$	$\frac{14845885397}{13312369039}$	$-\frac{11095738249}{17277571017}$	$\frac{492634981}{3636676981}$					
$\frac{403}{500}$	$\frac{20316989634}{6884860127}$	$-\frac{131394348499}{17824041302}$	$\frac{93322771834}{18669658777}$	$-\frac{1402876489}{3972101524}$	$\frac{995358996}{9938713297}$				
$\frac{843}{914}$	$-\frac{43201454579}{7612764793}$	$\frac{153411035633}{10624445625}$	$-\frac{41147039387}{4353523903}$	$\frac{10217626493}{9156996340}$	$-\frac{370981559}{13196923332}$	$\frac{225505817}{9209985516}$			
1	$\frac{54022175333}{5049238637}$	$-\frac{16168}{597}$	$\frac{80268235333}{4406197032}$	$-\frac{20772362192}{12387149319}$	$\frac{2266507289}{7017569123}$	$\frac{68547053}{9358646967}$	$\frac{228938958}{18303592411}$		
1	$\frac{724515903}{22886639447}$	0	$\frac{899615929}{5654603703}$	$\frac{613671907}{3560760024}$	$\frac{567482586}{5662882853}$	$\frac{545579326}{19135482045}$	$\frac{60463888}{7388418801}$	0	
b	$\frac{724515903}{22886639447}$	0	$\frac{899615929}{5654603703}$	$\frac{613671907}{3560760024}$	$\frac{567482586}{5662882853}$	$\frac{545579326}{19135482045}$	$\frac{60463888}{7388418801}$	0	0
b'	$\frac{724515903}{22886639447}$	0	$\frac{1280391897}{7151868092}$	$\frac{3155657169}{12133111769}$	$\frac{3457081385}{13745841103}$	$\frac{2223579981}{15129897557}$	$\frac{1384980154}{13146530033}$	$\frac{267013409}{10507265698}$	0
$\hat{b}$	$\frac{244089581}{6037832087}$	0	$\frac{1184541545}{8590099598}$	$\frac{2521567700}{12669817931}$	$\frac{323834586}{4537055981}$	$\frac{1782668550}{34202764021}$	$-\frac{7372963}{8771730113}$	0	0
$\hat{b}'$	$\frac{244089581}{6037832087}$	0	$\frac{1762709126}{11359523053}$	$\frac{1165689071}{3881131751}$	$\frac{2233493239}{12468443084}$	$\frac{1817122300}{6763577791}$	$-\frac{60456723}{5587273906}$	$-\frac{193034651}{2327874937}$	$\frac{3}{20}$

Table 4.4
Coefficients of $NEW8(6)P$ (rational approximations accurate to 20 digits).

0									
$\frac{302411531}{6408771185}$	$\frac{7653983}{6874962401}$								
$\frac{730332899}{7738687118}$	$\frac{6375199}{4294749553}$	$\frac{12750398}{4294749553}$							
$\frac{3}{10}$	$\frac{273434318}{5108325573}$	$-\frac{736290599}{6549499764}$	$\frac{192202107}{1850015270}$						
$\frac{5}{9}$	$-\frac{3921832152}{16243927381}$	$\frac{1237599120}{1875352829}$	$-\frac{5996145241}{16077216076}$	$\frac{496356401}{4562719032}$					
$\frac{10516905979}{15268622681}$	$\frac{10025761088}{17604369183}$	$-\frac{9286743615}{6180517933}$	$\frac{6665979450}{5752269941}$	$-\frac{408241474}{10823371237}$	$\frac{241166711}{4904581294}$				
$\frac{11577003015}{13271993539}$	$-\frac{516338243}{9672287701}$	$\frac{1832290931}{6277842291}$	$-\frac{18531011618}{129156819373}$	$\frac{2418431587}{11585848223}$	$\frac{1600299749}{42110091849}$	$\frac{386295139}{9983290553}$			
1	$-\frac{322739345}{9832418727}$	$-\frac{656762641}{5055440043}$	$\frac{11436849679}{26221526871}$	$\frac{13358015}{7831238438}$	$\frac{2661527991}{11234338420}$	$-\frac{4442333474}{81431247151}$	$\frac{529809481}{12462932631}$		
1	$\frac{180127983}{6831842764}$	0	$\frac{1296544255}{9243894812}$	$\frac{1728881303}{9941294262}$	$\frac{1548292225}{15658298817}$	$\frac{41546563}{1168504442}$	$\frac{95538361}{3816931135}$	0	
b	$\frac{180127983}{6831842764}$	0	$\frac{1296544255}{9243894812}$	$\frac{1728881303}{9941294262}$	$\frac{1548292225}{15658298817}$	$\frac{41546563}{1168504442}$	$\frac{95538361}{3816931135}$	0	0
b'	$\frac{180127983}{6831842764}$	0	$\frac{1911136913}{12339802434}$	$\frac{756091112}{3043336147}$	$\frac{5064499946}{22763849021}$	$\frac{733839751}{6423136863}$	$\frac{734562893}{3747974581}$	$\frac{462192311}{12292992462}$	0
$\hat{b}$	$\frac{158098118}{2604605623}$	0	$\frac{465929917}{7532645463}$	$\frac{1054420403}{3957866139}$	$-\frac{66519559}{3586531893}$	$\frac{596535105}{5015955652}$	$\frac{148581271}{13946053250}$	0	0
$\hat{b}'$	$\frac{158098118}{2604605623}$	0	$\frac{107258214}{1570385393}$	$\frac{11381575515}{29905269803}$	$-\frac{199558677}{4782042524}$	$\frac{5778730188}{15121705525}$	$\frac{303575179}{3639021511}$	$-\frac{1224440801}{14676786954}$	$\frac{3}{20}$

TABLE 5.1
NEW8(7)P against PD8(7)

log global error	G1	G2	G3	G4	G5	
-1						
-2	28			36		
-3	32	42	-2	44		
-4	35	38	-4	30	7	
-5	37	39	10	30	11	
-6	38	37	25	40	10	
-7					20	
-8					32	
-9						
	34	39	7	36	16	27%

Efficiency gains tables. Unity represents 1%. Numbers have been rounded to the nearest digit. Positive numbers mean that the first method is superior. The final row, gives the mean value of efficiency gain for all tolerances in a problem. The rightmost lower number is the average efficiency gain for all problems. Empty places in the tables are due to the unavailability of data for the respective tolerances.

problem G$'$1:

$$y''(x) = -25\, y(x), \quad y(0) = 1, \quad y'(0) = 0, \quad x \in [0, 1000].$$

and instead of G3 the wave equation described in [8] with $x \in [0, 1000]$ (referenced here as G$'$3). The class of problems G$'$ is thus defined as G$'$ = {G$'$1, G2, G$'$3, G4, G5}. We have found these problems to be representative of the type of periodic problems we are concerned here.

The compilation of the results of these tests is presented here (Tables 5.1, 5.3, 5.2, 5.4, and 5.5.) in the tabular format used also in [17] and [14] (we refer to the second of these references for a more detailed explanation of how exactly these numbers are derived). This format is based on the work of Enright and Pryce [5].

Studying the respective tables we see that all new pairs exhibit better performance than older pairs. Moreover, in all cases high phase-lag order pairs seem to perform, on this set of test problems, better than the general purpose pairs (either old or new ones).

6. APPENDIX: Algorithm for the construction of FSAL Nÿstrom pairs of orders 8(6)**.** Choose c_4, c_5, c_6, c_7, a_{82}, and $\hat{b}'_9$ as free parameters. Exclude those cases that could lead to indeterminate values on some of the following rational expressions. Set $c_8 = 1$, $b_2 = \hat{b}_2 = b'_2 = \hat{b}'_2 = 0$.

Estimate the remaining coefficients in the following order. Note that in some cases parallel paths may also be followed.

First set

$$\begin{aligned} d_1 &:= \left(7c_5\left(c_6\left(5c_7-3\right)-3c_7+2\right)-7c_6\left(3c_7-2\right)+2\left(7c_7-5\right)\right), \\ d_2 &:= \left(c_5\left(5c_6\left(2c_7-1\right)-5c_7+3\right)+c_6\left(3-5c_7\right)+3c_7-2\right), \end{aligned}$$

and estimate

$$c_3 = \frac{2c_4d_1-2c_5\left(7c_6\left(3c_7-2\right)-2\left(7c_7-5\right)\right)+4c_6\left(7c_7-5\right)-5\left(4c_7-3\right)}{2\left(7c_4d_2-7c_5\left(c_6\left(5c_7-3\right)-3c_7+2\right)+7c_6\left(3c_7-2\right)-2\left(7c_7-5\right)\right)},$$

Table 5.2
NEW6(4)P against DEP6(4)

log global error	G1	G2	G3	G4	G5	
-1	34	35		29		
-2	37	30	28	42		
-3	38	24	19	35	32	
-4	35	18	20	25	33	
-5	29	13	19	15	0	
-6	23	11	16	7	-2	
-7			13		-5	
-8					-5	
-9					-4	
	33	22	19	26	7	21%

Table 5.3
NEW4(3)P against DEP4(3)

log global error	G1	G2	G3	G4	G5	
-1	24					
-2	19	140		131		
-3	18	137	29	126	-45	
-4	18	141	33	131	-48	
-5	18	146	31	142	-39	
-6	18	151	28	153	-33	
-7					-32	
-8					-30	
-9						
	19	143	30	136	-40	58%

$c_2 = \dfrac{c_3}{2}$.

Next define

$$f_1(x) := (x(5c_6(2c_7-1)-5c_7+3)+c_6(3-5c_7)+3c_7-2),$$

and compute the following three weights

$$b'_3 = -\frac{7c_4 f_1(c_5) - 7c_5(c_6(5c_7-3)-3c_7+2)+7c_6(3c_7-2)-2(7c_7-5)}{420c_3(c_3-1)(c_3-c_4)(c_3-c_5)(c_3-c_6)(c_3-c_7)},$$

$$b'_4 = \frac{7c_3 f_1(c_5) - 7c_5(c_6(5c_7-3)-3c_7+2)+7c_6(3c_7-2)-2(7c_7-5)}{420c_4(c_3-c_4)(c_4-1)(c_4-c_5)(c_4-c_6)(c_4-c_7)},$$

$$b'_5 = -\frac{7c_3 f_1(c_4) - 7c_4(c_6(5c_7-3)-3c_7+2)+7c_6(3c_7-2)-2(7c_7-5)}{420c_5(c_3-c_5)(c_4-c_5)(c_5-1)(c_5-c_6)(c_5-c_7)}.$$

Define

$$f_2(x) := 12x(x-c_7)(x-1),$$

and find

$$b'_6 = -\frac{b'_3 f_2(c_3) + b'_4 f_2(c_4) + b'_5 f_2(c_5) - 2c_7 + 1}{12c_6(c_6-1)(c_6-c_7)},$$

$$b'_7 = -\frac{6b'_3c_3(c_3-1)+6b'_4c_4(c_4-1)+6b'_5c_5(c_5-1)+6b'_6c_6(c_6-1)+1}{6c_7(c_7-1)},$$

TABLE 5.4
NEW8(6) against DEP8(6). The comparison concerns the problems of class D of DETEST.

log global error	D1	D2	D3	D4	D5
−1					
−2					−12
−3			−5	7	−3
−4	−10	−8	6	11	5
−5	−10	−8	12	18	14
−6	−7	−3	16	27	23
−7	8	−3	19	28	32
−8	18	0	27	26	
−9	19	3	27		
−10	22	7			
	6	−2	14	19	10
					10%

TABLE 5.5
NEW8(6)P against NEW8(6)

log global error	G1	G2	G3	G4	G5
−1					
−2			17		
−3	27		19	18	
−4	34	27	10	20	1
−5	11	19	6	12	9
−6	9	13	11	11	15
−7	7	10	10	9	−16
−8	6	8	13	9	−11
−9	5	6	18	9	−8
−10					−5
	14	14	13	13	−2
					11%

$$b'_8 = -\frac{2b'_3c_3 + 2b'_4c_4 + 2b'_5c_5 + 2b'_6c_6 + 2b'_7c_7 - 1}{2c_8},$$
$$b'_1 = 1 - b'_3 - b'_4 - b'_5 - b'_6 - b'_7 - b'_8,$$
$$b_1 = b'_1,\quad b_3 = b'_3(1-c_3),\quad b_4 = b'_4(1-c_4),\quad b_5 = b'_5(1-c_5),\quad b_6 = b'_6(1-c_6),$$
$$b_7 = b'_7(1-c_7),\quad b_8 = b_9 = 0,$$
$$a_{32} = \frac{c_3^3}{6c_2},\quad a_{42} = -\frac{c_4^3(2c_3 - c_4)}{12c_2(c_2 - c_3)},\quad a_{43} = \frac{c_4^3(2c_2 - c_4)}{12c_3(c_2 - c_3)}.$$

Define

$$g(x,y,z) := x^2 - x(y+z) + yz,$$

to compute

$$a_{72} = -\frac{a_{32}b'_3g(c_3,c_5,c_6) + a_{42}b'_4g(c_4,c_5,c_6) + a_{82}b'_8(c_6-1)(c_5-1)}{b'_7(c_5-c_7)(c_6-c_7)},$$
$$a_{62} = \frac{a_{32}b'_3g(c_3,c_5,c_7) + a_{42}b'_4g(c_4,c_5,c_7) + a_{82}b'_8(c_7-1)(c_5-1)}{b'_6(c_5-c_6)(c_6-c_7)},$$
$$a_{52} = -\frac{a_{32}b'_3g(c_3,c_6,c_7) + a_{42}b'_4g(c_4,c_6,c_7) + a_{82}b'_8(c_7-1)(c_6-1)}{b'_5(c_5-c_6)(c_5-c_7)}.$$

Define

$$f_3(x) = (x - c_7)(x - 1),$$

set

$K_{11} = a_{32}c_2b_3' f_3(c_3) + a_{42}c_2b_4' f_3(c_4) + a_{52}c_2b_5' f_3(c_5) + a_{62}c_2b_6' f_3(c_6)$,

$K_{12} = -4c_3(7c_4(3c_7 - 2) - 7c_7 + 5) + 4c_4(7c_7 - 5) - 3(4c_7 - 3)$,

$K_{21} = a_{32}c_2b_3'(c_3 - 1) + a_{42}c_2b_4'(c_4 - 1) + a_{52}c_2b_5'(c_5 - 1) + a_{62}c_2b_6'(c_6 - 1) + a_{72}c_2b_7'(c_7 - 1)$,

$K_{22} = -2c_3(7c_4(3c_5 - 1) - 7c_5 + 3) + 2c_4(7c_5 - 3) - 3(2c_5 - 1)$,

$K_{31} = a_{32}c_2b_3'(c_3 - 1) + a_{42}c_2b_4'(c_4 - 1) + a_{52}c_2b_5'(c_5 - 1) + a_{62}c_2b_6'(c_6 - 1) + a_{72}c_2b_7'(c_7 - 1)$,

$K_{32} = a_{65}c_5b_6'(c_6 - 1)(c_5 - c_6)(c_4 - c_5)(c_3 - c_5) - 2c_3(7c_4(3c_6 - 1) - 7c_6 + 3) + 2c_4(7c_6 - 3) - 3(2c_6 - 1)$,

and substitute in

$$a_{65} = -\frac{10080K_{11}(c_2 - c_4)(c_2 - c_3) + K_{12}}{10080c_5b_6'(c_3 - c_5)(c_4 - c_5)(c_6 - 1)(c_6 - c_7)},$$

$$a_{76} = \frac{5040K_{21}(c_2 - c_5)(c_2 - c_4)(c_2 - c_3) + K_{22}}{5040c_6b_7'(c_3 - c_6)(c_4 - c_6)(c_5 - c_6)(c_7 - 1)},$$

$$a_{75} = -\frac{5040K_{31}(c_2 - c_6)(c_2 - c_4)(c_2 - c_3) + K_{32}}{5040c_5b_7'(c_3 - c_5)(c_4 - c_5)(c_5 - c_6)(c_7 - 1)}.$$

Then estimate the following coefficients

$$a_{53} = -\frac{12a_{52}c_2(c_2 - c_4) + c_5^3(2c_4 - c_5)}{12c_3(c_3 - c_4)},$$

$$a_{54} = \frac{12a_{52}c_2(c_2 - c_3) + c_5^3(2c_3 - c_5)}{12c_4(c_3 - c_4)},$$

$$a_{63} = -\frac{12a_{62}c_2(c_2 - c_4) - 12a_{65}c_5(c_4 - c_5) + c_6^3(2c_4 - c_6)}{12c_3(c_3 - c_4)},$$

$$a_{64} = \frac{12a_{62}c_2(c_2 - c_3) - 12a_{65}c_5(c_3 - c_5) + c_6^3(2c_3 - c_6)}{12c_4(c_3 - c_4)},$$

$$a_{73} = -\frac{12a_{72}c_2(c_2 - c_4) - 12a_{75}c_5(c_4 - c_5) - 12a_{76}c_6(c_4 - c_6) + c_7^3(2c_4 - c_7)}{12c_3(c_3 - c_4)},$$

$$a_{74} = \frac{12a_{72}c_2(c_2 - c_3) - 12a_{75}c_5(c_3 - c_5) - 12a_{76}c_6(c_3 - c_6) + c_7^3(2c_3 - c_7)}{12c_4(c_3 - c_4)},$$

$$a_{83} = -\frac{2a_{43}b_4' + 2a_{53}b_5' + 2a_{63}b_6' + 2a_{73}b_7' - b_3'\left(c_3^2 - 2c_3 + 1\right)}{2b_8'},$$

$$a_{84} = -\frac{2a_{54}b_5' + 2a_{64}b_6' + 2a_{74}b_7' - b_4'\left(c_4^2 - 2c_4 + 1\right)}{2b_8'},$$

$$a_{85} = -\frac{2a_{65}b_6' + 2a_{75}b_7' - b_5'\left(c_5^2 - 2c_5 + 1\right)}{2b_8'},$$

$$a_{86} = -\frac{2a_{76}b_7' - b_6'\left(c_6^2 - 2c_6 + 1\right)}{2b_8'}, \quad a_{87} = \frac{b_7'(c_7 - 1)^2}{2b_8'}.$$

Estimate $\hat{b}_1'$, $\hat{b}_3'$, $\hat{b}_4'$, …, $\hat{b}_8'$ from $\hat{b}'e = 1$, $\hat{b}'c = \frac{1}{2}$, …, $\hat{b}'c^5 = \frac{1}{6}$ and $\hat{b}'AC^2c = \frac{1}{4 \cdot 5 \cdot 6}$ (Linear System), where $C = \operatorname{diag}(c)$.

Finally set $\hat{b}_1 = \hat{b}_1'$, $\hat{b}_3 = \hat{b}_3'(1 - c_3)$, $\hat{b}_4 = \hat{b}_4'(1 - c_4)$, $\hat{b}_5 = \hat{b}_5'(1 - c_5)$, $\hat{b}_6 = \hat{b}_6'(1 - c_6)$, $\hat{b}_7 = \hat{b}_7'(1 - c_7)$, $\hat{b}_8 = \hat{b}_9 = 0$.

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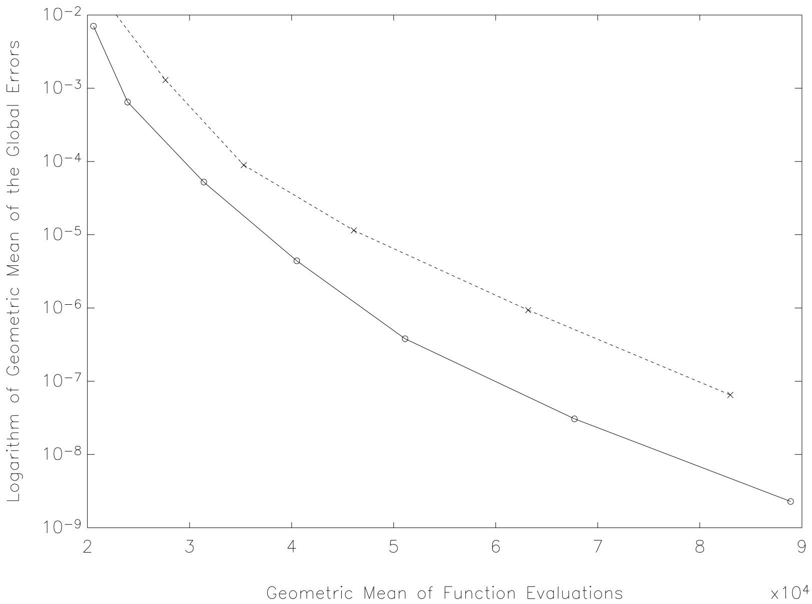

FIG. 7.1. *NEW8(7)P — against PD8(7) - - - on the problems of class G.*

7. APPENDIX: Additional numerical evaluation. Another interpretation of the tests of Section 5 is presented here. This second format is that of the graphical representation of the geometric mean of the maximum global errors over the whole integration interval, for all problems in each case $\left(\prod_{i=1}^{5} ge_{i,TOL}\right)^{1/5}$, against the geometric mean of the cost in function evaluations $\left(\prod_{i=1}^{5} fe_{i,TOL}\right)^{1/5}$ for each tolerance. We prefer this type of graphical representation for reasons explained in [10], [14]. These are presented in Figures 7.1, 7.2, 7.3, 7.4, and 7.5. In practice, we have found that both the tabular and graphical type of representation of the above comparisons lead virtually at the same quantitative overall picture.

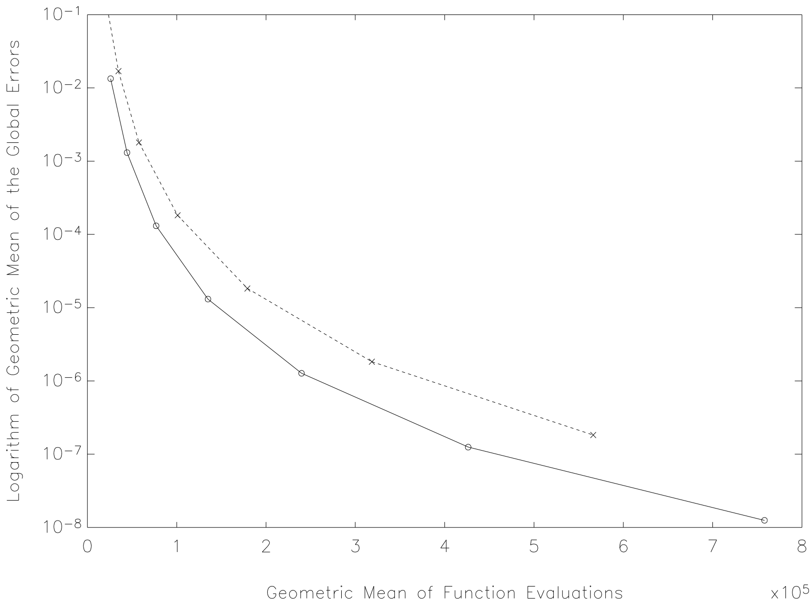

FIG. 7.2. *NEW4(3)P — against DEP4(3) - - - on the problems of class G′.*

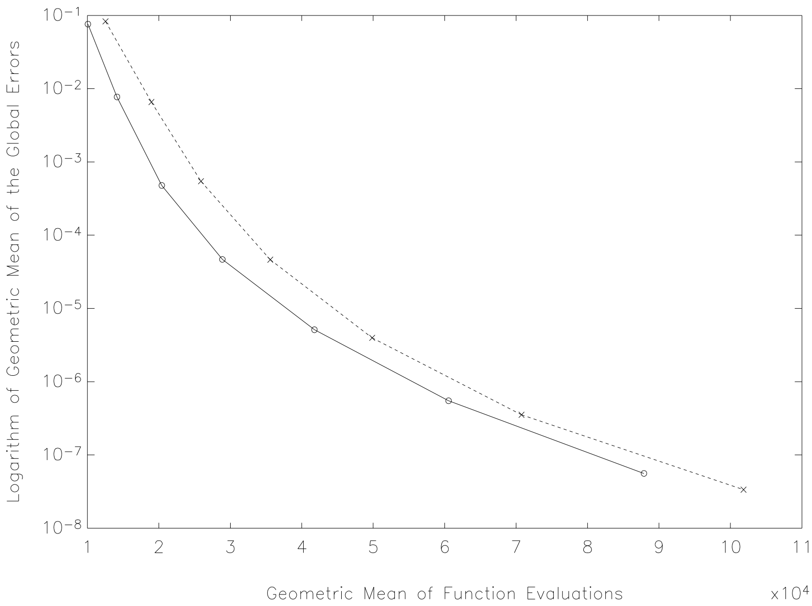

FIG. 7.3. *NEW6(4)P — against DEP6(4) - - - on the problems of class G′.*

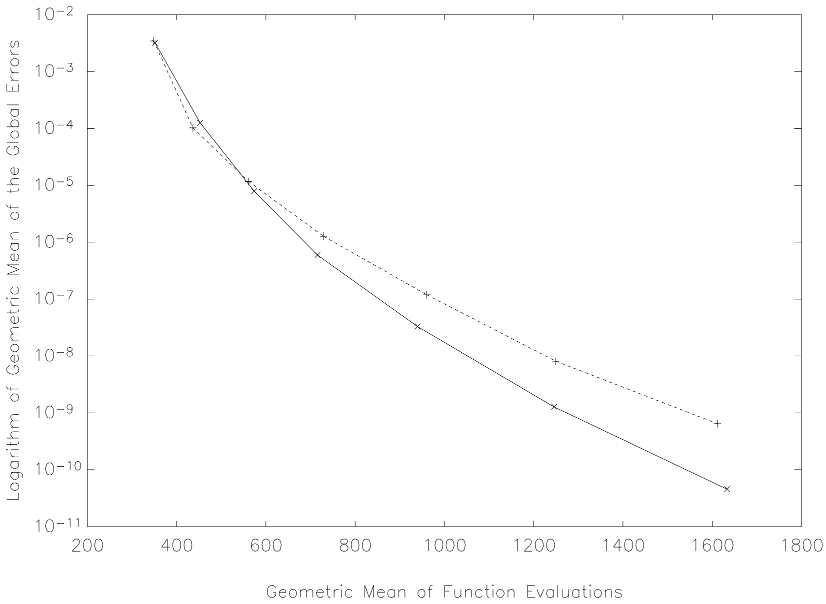

FIG. 7.4. *NEW8(6) — against DEP8(6) - - - on the problems of class D of DETEST.*

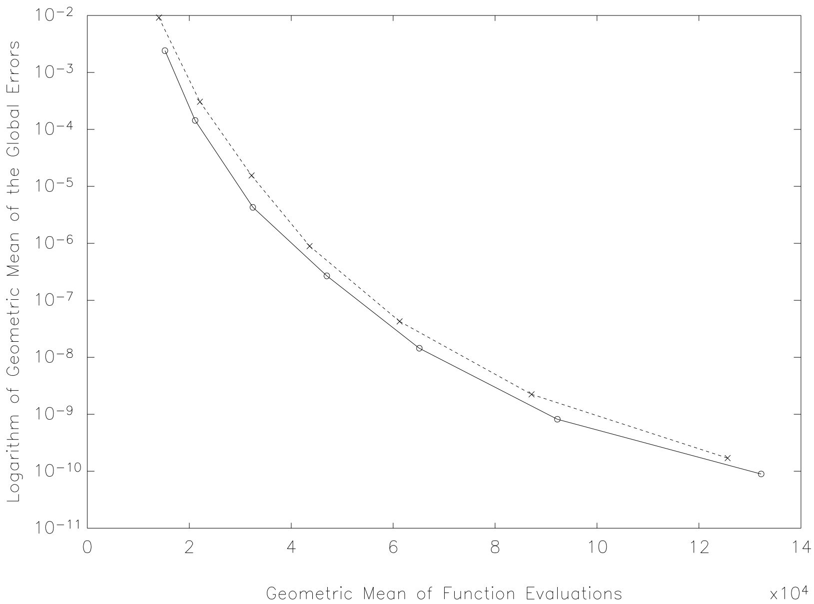

FIG. 7.5. *NEW8(6)P — against NEW8(6) - - - on the problems of class G′.*