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HYBRID METHODS FOR A SPECIAL CLASS OF SECOND-ORDER DIFFERENTIAL EQUATIONS

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Abstract

Hybrid methods for the numerical solution of second order ordinary differential equations not containing y' are developed. The order p of such stable k-step methods is not limited to $p = k + 1$ $(k + 2)$. The customary linear k-step schemes are modified by including the values of the second derivative at one "offstep" point. It is shown that the order of these hybrid methods is not subject to the above restrictions. Numerical experiments are presented. It is shown that the maximal order is achieved.

§1. Introduction

In this paper we are interested in developing direct methods for the numerical solution of a special class of second-order ordinary differential equation, namely

$$y''(x) = f(x,y(x)). \tag{1}$$

There exist methods of Runge-Kutta type which tackle this problem directly (Collatz [2, p.61], de Vogelaere [9], Scraton [8]) and linear k-step methods of the form

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h^2 \sum_{j=0}^{k'} \beta_j f_{n+j} \tag{2}$$

(Henrici [6, p.289], Lambert [7, p.252]).

The direct application of methods of class (2) to problem (1), rather than the application of a conventional linear multistep method to an equivalent first-order system is usually recommended. Ash [1] studied asymptotic errors by both approaches, for a subclass of methods, and finds theoretical backing for this recommendation.

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A rigid theory of the stability and convergence of general multistep methods was developed by Dahlquist [3,4] and Henrici [6, p.307]. The following two notions are basic in this theory.

Let $\rho(\xi)$, $\sigma(\xi)$, the first and second characteristic polynomials of the linear multistep method (2) be defined by

$$\rho(\xi) = \sum_{j=0}^{k} \alpha_j \xi^j \tag{3}$$

$$\sigma(\xi) = \sum_{j=0}^{k'} \beta_j \xi^j . \tag{4}$$

Definition 1: The method (2) is said to be zero-stable if no root of th first characteristic polynomial $\rho(\xi)$ has modulus greater than one, and i every root of modulus one has multiplicity not greater than two.

Definition 2: The method (2) has order p if the linear difference operator

$$L[y(x);h] = \sum_{j=0}^{k} \alpha_j y(x+jh) - h^2 \sum_{j=0}^{k'} \beta_j y''(x+jh), \tag{5}$$

where $y(x)$ is an arbitrary function, can be expanded in Taylor's series as follows

$$L[y(x);h] = C_{p+2} h^{p+2} y^{(p+2)}(x) + O(h^{p+3}) \tag{6}$$

and $C_{p+2} \neq 0$. The number C_{p+2} is called the error constant.

Definition 3: The method (2) is said to be consistent if it has order a least one.

One can easily show that for a consistent method

$$\rho(1) = \rho'(1) = 0, \tag{7}$$

$$\rho''(1) = 2\sigma(1). \tag{8}$$

Theorem 1 (Henrici [6, p.307]):

The order p of a zero-stable method (2) cannot exceed k+2. A necessary and sufficient condition for $p = k+2$ is that k be even, that all roots of $\rho(\xi)$ have modulus one, and that $\sigma(\xi)$ be determined by

$$\sigma(\xi) = \sum_{j=0}^{k'} c_j (\xi-1)^j \tag{9}$$

and c_j are the coefficients in the expansion of

$$\frac{\rho(\xi)}{(\log \xi)^2} = \sum_{j=0}^{\infty} c_j (\xi-1)^j . \tag{10}$$

Since stability is a necessary condition for convergence, the last theorem restricts the order of multistep methods for larger k. Although $p = 2k - 1$ could actually be attained if both ρ and σ were chosen judiciously (there are $2k + 1$ independent parameters, see [3]), one has to confine oneself to the use of schemes with $p = k + 1$ (or $k + 2$) to have convergence. According to the previous theorem the only way to stable methods of higher order lies in a modification of the method (2).

The approach to a relaxation of the previous theorem is similar to that of Gragg and Stetter [5]. We include in (2) the second derivative at a single offstep point x_{n+r}, with a real $r \notin I_k := \{0,1,\ldots,k\}$, usually noninteger. The values of $f(x,y)$ at the point x_{n+r} - and at x_{n+k} if necessary - are predicted as usual. Since $f(x_{n+r},y^*_{n+r})$ is not needed in further steps it requires no correction. Details are given in the next section.

For a given ρ, the generalized k-step method with a σ of degree k' is normally of order $p \geq k' + 3$. Even more striking is it, however, that the attempt to utilize the full number of $k + k' + 2$ independent parameters for the construction of schemes of maximal order succeeds without destroying stability.

In the next section the generalized algorithms are described. Section 3 will be devoted to construction of optimal order algorithms for which the first charactersitic polynomial, ρ, is given. Some examples are given. In section 4 we discuss the construction of optimal stable algorithms and give some examples. It is shown that such algorithms do not exist for 2-step method. In the last section we present some of the numerical experiments performed. These experiments show that the order is achieved.

§2. The Generalized Algorithms

The basis of our hybrid algorithms is the k-step difference operator (1.5). This operator can be written in the form

$$L[y(x);h]: = \rho(E)y(x) - h^2\sigma(E)y''(x) - h^2\beta_r E^r y''(x), r \notin I_k \qquad (1)$$

where the translation operator E is given by

$$Ey(x) = y(x+h); \qquad (2)$$

ρ is a polynomial of degree k and σ one of degree $k' \leq k$.

Predictors are used to obtain approximations to the values of the derivative at x_{n+r} and also at x_{n+k} if $k' = k$. Let $\rho^*, \hat{\rho}, \sigma^*$ and $\hat{\sigma}$ be suitable polynomials of degree k-1 and $\bar{\rho}$ and $\bar{\sigma}$ the polynomials of degree k-1 for which $\rho(z) = \alpha_k z^k - \bar{\rho}(z), \alpha_k \neq 0$; $\sigma(z) = \beta_k z^k + \bar{\sigma}(z)$. Assuming the necessary initial data $y_m, f_m^* = f_m = f(x_m, y_m)$ $m = 0,1,\ldots,k-1$, are known, we have the following algorithms

I. $k' < k$ Explicit Hybrid Method (EHM)

$$(P_r)\ \hat{f}_{n+r}: = f(x_{n+r}, \hat{\rho}(E)y_n + h^2\, \hat{\sigma}(E)f_n),$$

$$(C)\ y_{n+k}: = \bar{\rho}(E)y_n + h^2\, \bar{\sigma}(E)f_n + h^2\, \beta_r \hat{f}_{n+r},$$

$$(C_f)\ f_{n+k}: = f(x_{n+k}, y_{n+k});$$

II. $k' = k$ Implicit Hybrid Method (IHM)

$$(P_k)\ f^*_{n+k}: = f(x_{n+k}, \rho^*(E)y_n + h^2\, \sigma^*(E)f_n),$$

$$(P_r)\ \hat{f}_{n+r}: = f(x_{n+r}, \hat{\rho}(E)y_n + h^2\, \hat{\sigma}(E)f_n),$$

$$(C)\ y_{n+k}: = \bar{\rho}(E)y_n + h^2\, \bar{\sigma}(E)f_n + h^2\, \beta_k f^*_{n+k} + h^2\beta_r \hat{f}_{n+r},$$

$$(C_f)\ f_{n+k}: = f(x_{n+k}, y_{n+k});$$

III. $k' = k$ Simplified Implicit Hybrid Method (SIHM)

$$(P_k)\quad f^*_{n+k} := f(x_{n+k}, \rho^*(E)y_n + h^2\sigma^*(E)f_n^*),$$

$$(P_r)\quad f_{n+r} := f(x_{n+r}, \hat{\rho}(E)y_n + h^2\hat{\sigma}(E)f_n^*),$$

$$(C)\quad y_{n+k} := \bar{\rho}(E)y_n + h^2\sigma(E)f_n^* + h^2\beta_r\hat{f}_{n+r}.$$

Algorithm III omits the correction step (C_f) of the predicted value of f.

In the last section we discuss the choice of the characteristic polynomials $\hat{\rho}, \hat{\sigma}, \rho^*$ and σ^*.

We now turn to the construction of stable operators (1) which are of optimal order of accuracy.

§3. Optimal Order Algorithms with given ρ

The following development follows largely the theory of [6].

Lemma 2: (1.6) is equivalent to

$$\frac{\rho(\zeta)}{(\log\zeta)^2} - \sigma(\zeta) - \beta_r\zeta^r = C_{p+2}(\zeta-1)^p + O((\zeta-1)^{p+1}). \tag{1}$$

Proof: Express the translation operator E by the exponential of the differentiation operator $\partial(\partial y(x) := y'(x))$. Then the following is equivalent to (1.6):

$$\rho(e^{h\partial}) - h^2\partial^2[\sigma(e^{h\partial}) + \beta_r e^{h\partial r}] = C_{p+2}h^{p+2}\partial^{p+2} + O(h^{p+3}). \tag{2}$$

Let ζ be defined by

$$h\partial : \log\zeta = \log(1 + (\zeta-1)). \tag{3}$$

Thus

$$\rho(\zeta) - (\log\zeta)^2[\sigma(\zeta) + \beta_r\zeta^r] = C_{p+2}(\log\zeta)^{p+2} + O(h^{p+3}). \tag{4}$$

Dividing by $(\log\zeta)^2$ and using the Taylor expansion of $\log\zeta$

$$\log\zeta = \sum_{i=0}^{\infty} \frac{(\zeta-1)^i}{i}(-1)^{i-1} \tag{5}$$

one obtains (1).

Corollary (Consistency conditions): For $p \geq 1$ it is necessary that

$$\rho(1) = \rho'(1) = 0, \tag{6}$$

$$\rho''(1) = 2\sigma(1) + 2\beta_r. \tag{7}$$

Note that the second condition differs slightly from the usual condition $\rho''(1) = 2\sigma(1)$.

Let's use the following notations:

$$\rho(\zeta) = \sum_{j=0}^{k} \alpha_j \zeta^j = \sum_{j=2}^{k} a_j (\zeta-1)^j \tag{8}$$

$$\sigma(\zeta) = \sum_{j=0}^{k'} \beta_j \zeta^j = \sum_{j=0}^{k'} b_j (\zeta-1)^j \tag{9}$$

$$\frac{\rho(\zeta)}{(\log \zeta)^2} = \sum_{j=0}^{\infty} d_j (\zeta-1)^j \tag{10}$$

with

$$d_j = \sum_{i=0}^{\min(j,k-2)} a_{i+2}\delta_{j-i} \tag{11}$$

where

$$\delta_j = \sum_{i=0}^{j} \gamma_i \gamma_{j-i} \tag{12}$$

and

$$\frac{\zeta-1}{\log \zeta} := \sum_{i=0}^{\infty} \gamma_i (\zeta-1)^i. \tag{13}$$

A table of values of γ_i, δ_i computed in quadruple precision on ITEL AS/6 computer follows:

i	C_i	D_i
0	0.1000000000000Q+01	0.1000000000000Q+01
1	0.5000000000000Q+00	0.1000000000000Q+01
2	-0.8333333333333Q-01	0.8333333333333Q-01
3	0.4166666666667Q-01	0.5777789833162Q-33
4	-0.2638888888889Q-01	-0.4166666666667Q-02
5	0.1875000000000Q-01	0.4166666666667Q-02
6	-0.1426917989418Q-01	-0.3654100529101Q-02
7	0.1136739417989Q-01	0.3141534391534Q-02
8	-0.9356536596120Q-02	-0.2708608906526Q-02
9	0.7892554012346Q-02	0.2355324074074Q-02
10	-0.6785849984635Q-02	-0.2067782237053Q-02
11	0.5924056412338Q-02	0.1832085738336Q-02
12	-0.5236693257950Q-02	-0.1636938285923Q-02
13	0.4677498407042Q-02	0.1473644952946Q-02
14	-0.4214952239005Q-02	-0.1335601777436Q-02
15	0.3826899553212Q-02	0.1217785362105Q-02
16	-0.3497349845350Q-02	-0.1116346064718Q-02
17	0.3214496431324Q-02	0.1028304779072Q-02
18	-0.2969447715458Q-02	-0.9513317383875Q-03
19	0.2755390299437Q-02	0.8835857729287Q-03
20	-0.2567022545007Q-02	-0.8235970347234Q-03
21	0.2400162378591Q-02	0.7701807833231Q-03
22	-0.2251470197759Q-02	-0.7223734188781Q-03
23	0.2118249527295Q-02	0.6793845524365Q-03
24	-0.1998301255043Q-02	-0.6405607345004Q-03
25	0.1889815463679Q-02	0.6053577377107Q-03
26	-0.1791290078072Q-02	-0.5733191764914Q-03
27	0.1701468926370Q-02	0.5440598661754Q-03
28	-0.1619294049096Q-02	-0.5172527600200Q-03
29	0.1543868596928Q-02	0.4926186116083Q-03
30	-0.1474427689061Q-02	-0.4699177312257Q-03
31	0.1410315320613Q-02	0.4489433643643Q-03
32	-0.1350965912313Q-02	-0.4295163367065Q-03
33	0.1295889455825Q-02	0.4114806952918Q-03
34	-0.1244659468109Q-02	-0.3947001388135Q-03
35	0.1196903157952Q-02	0.3790550772309Q-03
36	-0.1152293347826Q-02	-0.3644401964550Q-03
37	0.1110541798418Q-02	0.3507624308518Q-03
38	-0.1071393661517Q-02	-0.3379392669331Q-03
39	0.1034622846280Q-02	0.3258973174791Q-03
40	-0.1000028129257Q-02	-0.3145711176325Q-03
41	0.9674298734228Q-03	0.3039021040964Q-03
42	-0.9366672485568Q-03	-0.2938877460843Q-03
43	0.9075958663861Q-03	0.2843308026127Q-03
44	-0.8800857605299Q-03	-0.2753386854306Q-03
45	0.8540196543670Q-03	0.2668229106396Q-03
46	-0.8292914703794Q-03	-0.2587486250710Q-03
47	0.8058050428514Q-03	0.2510841959113Q-03
48	-0.7834730024921Q-03	-0.2438008540341Q-03
49	0.7622158069591Q-03	0.2368723830940Q-03
50	-0.7419608956387Q-03	-0.2302748477415Q-03

Table 1

For many considerations it will prove advantageous to use the transformation

$$\zeta = \frac{1+z}{1-z}, \quad z = \frac{\zeta - 1}{\zeta + 1}, \tag{14}$$

and to regard the polynomials

$$R(z) := \left(\frac{1-z}{2}\right)^k \rho\left(\frac{1+z}{1-z}\right) = \sum_{j=2}^{k} A_j z^j \tag{15}$$

$$S(z) := \left(\frac{1-z}{2}\right)^k \sigma\left(\frac{1+z}{1-z}\right) = \sum_{j=0}^{k} B_j z^j \tag{16}$$

$$T_k(z,r) := \left(\frac{1-z}{2}\right)^k \left(\frac{1+z}{1-z}\right)^r =: \sum_{i=0}^{\infty} P_j^{\,k}(r) z^j \tag{17}$$

$$\frac{R(z)}{\left(\log\left(\frac{1+z}{1-z}\right)\right)^2} = \sum_{j=0}^{\infty} D_j z^j \tag{18}$$

with

$$D_j = \sum_{i=\max(0,[(j-k+1)/2]+1)}^{[j/2]} \Gamma'_{2i} A_{j-2i+2} \tag{19}$$

where

$$\Gamma'_{2j} = \sum_{i=0}^{j} \Gamma_{2i} \Gamma_{2(j-i)}, \tag{20}$$

and

$$\frac{2z}{\log\left(\frac{1+z}{1-z}\right)} =: \sum_{j=0}^{\infty} \Gamma_{2j} z^{2j}. \tag{21}$$

A table of values of Γ_i, Γ'_i computed in quadruple precision on ITEL AS/6 computer follows:

i	Γ_i	Γ_i'
0	0.500000000000Q+00	0.250000000000Q+00
2	-0.166666666667Q+00	-0.166666666667Q+00
4	-0.444444444444Q-01	-0.166666666667Q-01
6	-0.232804232804Q-01	-0.846560846560Q-02
8	-0.150970017636Q-01	-0.536155202821Q-02
10	-0.108984020095Q-01	-0.379669713003Q-02
12	-0.839377592816Q-02	-0.287704143788Q-02
14	-0.675138252563Q-02	-0.228178118830Q-02
16	-0.560187281885Q-02	-0.186994027516Q-02
18	-0.475803659726Q-02	-0.157073506470Q-02
20	-0.411560328367Q-02	-0.134507988182Q-02
22	-0.361223236869Q-02	-0.116979132359Q-02
24	-0.320853151569Q-02	-0.103032744078Q-02
26	-0.287847722314Q-02	-0.917147141228Q-03
28	-0.260423782918Q-02	-0.823754595278Q-03
30	-0.237321534643Q-02	-0.745588170688Q-03
32	-0.217627506149Q-02	-0.679359070178Q-03
34	-0.200664373400Q-02	-0.622641842069Q-03
36	-0.185920054121Q-02	-0.573612139916Q-03
38	-0.173000733373Q-02	-0.530873797150Q-03
40	-0.161598942739Q-02	-0.493341839901Q-03
42	-0.151471377078Q-02	-0.460161533119Q-03
44	-0.142423167804Q-02	-0.430651222990Q-03
46	-0.134296532582Q-02	-0.404261247045Q-03
48	-0.126962450720Q-02	-0.380543911718Q-03
50	-0.120314468113Q-02	-0.359131231464Q-03

Table II

The fact that

$$\Gamma_{2i} < 0 \quad \text{for } i \geq 1 \tag{22}$$

was proved in [3]. It is evident from table 2 that

$$\Gamma'_{2i} < 0 \quad \text{for } i \geq 1. \tag{23}$$

(23) implies

$$\Gamma'_0 + \sum_{i=0}^{M} \Gamma'_{2i} > 0 \quad \text{for } M \geq 1 \tag{24}$$

since

$$\lim_{M\to\infty} \sum_{i=0}^{M} \Gamma_{2i} = 0.$$

<u>Lemma 3</u>: (1.6) is equivalent to

$$\frac{R(z)}{[\log(\frac{1+z}{1-z})]^2} - S(z) - \beta_r T_k(z;r) = 2^{p-k} D_{p+2} z^p + O(z^{p+1}). \tag{25}$$

<u>Proof:</u> By transforming equation (1) and observing that

$$\zeta - 1 = \frac{2z}{1-z} = 2z(1+z+\ldots) \tag{26}$$

the assertion follows.

One reason for the transormation (14) is

<u>Lemma 4</u> (Henrici [6, pp.305-306]):
For ρ to be stable it is necessary that

$$A_2 \neq 0; \; A_i A_2 \geq 0 \quad \text{for } i = 3,4,\ldots,k. \tag{27}$$

We will usually use $A_2 = 1$ as a normalization and use (27) in the form $A_i \geq 0$ for $i = 3,4,\ldots,k$.

The next lemma concerning the properties of $P_i^k(r)$ of the expansion (17) and

$$\bar{P}^k(r) = \sum_{i=0}^{k} P_i^k(r) \tag{28}$$

was proved in [5].

<u>Lemma 5</u> (Gragg and Stetter [5, p.193]):

$\bar{P}^k$ and P_i^k have the following properties:

(1) $\bar{P}^k$ is a polynomial of degree k; P_i^k is a polynomial of degree i.

(2) $P_i^k(k-r) = (-1)^i P_i^k(r)$.

(3) $\bar{P}^k(r) = 0$ for $r = 0,1,\ldots,k-1$,

$\bar{P}^k(r) > 0$ for $r > k - 1$,

$P_i^k(r) = 0$ for $r = 0,1,\ldots k$, $i \geq k + 1$,

$P_i^k(r) > 0$ for $r > k$, $i \geq k + 1$.

(4) For even $i - k > 0$, P_i^k has an additional zero at $i = k/2$.

(5) $\bar{P}^k(k) = 1$,

$P_i^k(k + 1) = 2$ for $i \geq k + 1$

(6) $\bar{P}^k(r) = \binom{r}{k}$, $P_{k+1}^k(r) = 2\binom{r}{k+1}$, $P_{k+2}^k(r) = 2\binom{r}{k+1}\frac{2r-k}{k+2}$.

(7) For $i \geq k + 1$, each P_i^k is a polynomial multiple of $\bar{P}^k$ and of P_{k+1}^k. Each P_i^k with even $i - k > 0$ is a polynomial multiple of P_{k+2}^k.

<u>Definition 4</u>: A polynomial is called <u>admissible</u> for k' if it is of degree $k \geq k'$ and if the coefficients d_i in (11) satisfy

$$d_{k'+1} \neq 0,$$

$$(k' + 2)\, d_{k'+2} + m d_{k'+1} \neq 0 \quad \text{for } m = 1,2,\ldots,k' + 1 \tag{29}$$

<u>Theorem 6</u>: Let ρ be a polynomial admissible for k' and let $\rho(1)=\rho'(1)=0$. Then there exist uniquely a polynomial σ of degree k', a constant β_r and a real number $r \notin I_k$, such that the order p of the corresponding operator L satisfies $p \geq k' + 3$.

<u>Proof</u>: By lemma 2 it must be shown that σ, β_r and $r \notin I_k$, can be chosen such that

$$d_j = b_j + \beta_r \binom{r}{j}, \quad j = 0,1,\ldots,k', \tag{30}$$

$$d_{k'+1} = \beta_r \binom{r}{k'+1} \quad , \tag{31}$$

$$d_{k'+2} = \beta_r \binom{r}{k'+2} \quad . \tag{32}$$

Since $d_{k'+1} \neq 0$ by hypothesis, we have from (31) - (32) that

$$r = k' + 1 + \frac{d_{k'+2}}{d_{k'+1}} (k' + 2) \notin I_{k'} \ . \tag{33}$$

This implies that $\binom{r}{k'+1} \neq 0$; hence

$$\beta_r = \frac{d_{k'+1}}{\binom{r}{k'+1}} \tag{34}$$

The b_j (and thus σ) are determined from (30).

<u>Examples</u>

I. Generalized Störmer-Cowell methods: $\rho(\zeta) = \zeta^k - 2\zeta^{k-1} + \zeta^{k-2}$.

From $\rho(\zeta) = \zeta^{k-2}(\zeta-1)^2 = \sum_{i=0}^{k-2} \binom{k-2}{i}(\zeta-1)^{i+2}$ we have

$$d_j = \sum_{i=0}^{\min(j,k-2)} \delta_{j-i} \binom{k-2}{i} .$$

From (29) - (33) we obtain, e.g., the following corrector:
$k=3$, $k'=2$, $r=2.8$, $\beta_r=.1240079$

$$y_{n+3} - 2y_{n+2} + y_{n+1} = h^2(-.0059524\, f_n + .1111111\, f_{n+1} + .7708334\, f_{n+2} + .1240079\, f_{n+2.8}) \tag{35}$$

$p \geq 5$

Note: If $k=2$, $k'=1$ then $d_3=0$ and the polynomial is not admissible. If $k=k'=2$ then $r=2$ and again the polynomial is not admissible.

II. Arbitrary stable ρ for $k=3$:

$$\rho(\zeta) = (\zeta-1)^2(a_2-a_3+a_3\zeta)$$

with

$$0 < \frac{a_2}{a_3} < 2 \tag{36}$$

a) $k' = 2$,

$$d_0 = a_2\delta_0 = a_2$$

$$d_1 = a_2\delta_1 + a_3\delta_0 = a_2 + a_3$$

$$d_2 = a_2\delta_2 + a_3\delta_1 = \frac{a_2}{12} + a_3$$

$$d_3 = a_2\delta_3 + a_3\delta_2 = \frac{a_3}{12}$$

$$d_4 = a_2\delta_4 + a_3\delta_3 = -\frac{a_2}{240}$$

$$r = 3 + 4\frac{d_4}{d_3} = 3 - \frac{a_2}{5a_3} \quad \Rightarrow \quad \frac{a_2}{5a_3} \neq 1, 2, 3 \tag{37}$$

$$\beta_r = \frac{d_3}{\binom{r}{3}}$$

$$b_0 = a_2 - \beta_r$$

$$b_1 = a_2 + a_3 - r\beta_r$$

$$b_2 = \frac{1}{12} a_2 + a_3 - \frac{r(r-1)}{2} \beta_r$$

If we let $a_2 = \frac{1}{2}$, $a_3 = 1$ (These satisfy (36), (37)), then

$$r = 2.9, \quad \beta_r = .1008267$$

$$b_0 = .5 - .1008267 = .3991733$$

$$b_1 = 1.5 - 2.9 \cdot .1008267 = 1.2076026$$

$$b_2 = \frac{1}{24} + 1 - \frac{2.9 \cdot 1.9}{2} .1008267 = .7638891$$

$\beta_0 = -.0445402$, $\beta_1 = -.3201756$, $\beta_2 = .7638891$

$\alpha_0 = -.5$, $\alpha_1 = 2$, $\alpha_2 = -2.5$, $\alpha_3 = 1$

$$y_{n+3} - 2.5\, y_{n+2} + 2\, y_{n+1} - .5\, y_n = h^2(-.0445402\, f_n - .3201756\, f_{n+1} + .7638891\, f_{n+2} + .1008267\, f_{n+2.9}).$$

$p \geq 5$

b) $k' = 3$

$$d_5 = a_2\delta_5 + a_3\delta_4 = (a_2 - a_3)\frac{1}{240}$$

$$r = 4 + 5\,\frac{a_3 - a_2}{a_2} = 5\,\frac{a_3}{a_2} - 1$$

Let $a_2 = 1.5$, $a_3 = 1$ then $r = \frac{7}{3}$, $\beta_r = .2169642$

$\therefore$ $b_0 = 1.2830358$, $b_1 = 1.9937502$, $b_2 = .7875002$, $b_3 = .0458334$,

$\beta_0 = .0309524$, $\beta_1 = .55625$, $\beta_2 = .641$, $\beta_3 = .04858334$,

$\alpha_0 = .5$, $\alpha_1 = 0$, $\alpha_2 = -1.5$, $\alpha_3 = 1$.

$$y_{n+3} - 1.5\, y_{n+2} + .5\, y_n = h^2 (.0309524\, f_n + .55625\, f_{n+1}$$
$$+ .641\, f_{n+2} + .0458334\, f_{n+3} + .2169642\, f_{n+7/3})$$

$p \geq 6$.

Note: For k = 2 the polynomial is not admissible as in case I.

§4. Optimal Stable Algorithms

For k > 2, we now try to construct stable operators L of any order $p = k' + k + 1$, this being the maximum value to be expected with $k' + k + 2$ independent parameters.

Extending the approach of the previous section, one could try to choose r such that the k linear equations for $a_2,\ldots,a_k,\beta_r$,

$$d_j - \beta_r\binom{r}{j} = \sum_{i=0}^{k-2} a_{i+2}\delta_{j-i} - \binom{r}{j}\beta_r = 0,\ j = k'+1,\ldots,k'+k \quad (1)$$

have a nontrivial solution. The determinant of (1) is a polynomial of degree $k' + k$ in r which has the $k' + 1$ trivial zeros $r = 0,1,\ldots,k'$ leading to $\beta_r \neq 0$, all $a_i = 0$. The remaining real zeros, if any, could be tested as to whether they produce a stable ρ or not. This straightforward method becomes quite complicated even for small values of k.

We would like to describe a method based on the transformation (3.14) and lemma 4.

According to lemma 3, consider the relations

$$B_i + \beta_r P_j^k(r) = D_j,\ j = 0,1,\ldots,k, \quad (2)$$

$$\beta_r P_{k+i}^k(r) = D_{k+i},\ i = 1,2,\ldots,k, \quad (3)$$

where the D_i are the linear combinations (3.19) of the A_i.

If $k' = k$, it is sufficient to regard (3) only, since (2) can then be satisfied by choosing the B_j accordingly and $S(z)$ generates a polynomial $\sigma(\zeta)$ of degree k:

$$\sigma(\zeta) = (\zeta + 1)^k \, S\left(\frac{\zeta - 1}{\zeta + 1}\right) = \sum_{i=0}^{k} B_i(\zeta - 1)^i(\zeta + 1)^{k-i}. \tag{4}$$

If $k' = k - 1$, S has to satisfy $S(1) = \sum_{i=0}^{k} B_i = 0$. Therefore we add all equations (2) and obtain another equation of the type (3):

$$\beta_r \bar{P}^k(r) = \sum_{i=0}^{k} D_i =: \bar{D}_k. \tag{5}$$

Hence we will in each case consider a system of k linear equations for $A_2, \ldots, A_k, \beta_r$, consisting of either (3) for $i = 1,2,\ldots,k$ or of (5) and (3) for $i = 1,2,\ldots,k-1$.

Note that for a stable ρ whose zeros are not all on the unit circle

$$D_{k+i} < 0 \quad \text{for } i = 1,2,\ldots \tag{6}$$

and

$$\bar{D}_k > 0. \tag{7}$$

(6) follows immediately from (3.19), (3.23) and lemma 4, while (7) requires also (3.24). From lemmas 5,6, we have the <u>necessary condition for stability</u>

$$\frac{k}{2} < r < \begin{cases} \infty & \text{if } k' = k, \\ k & \text{if } k' = k - 1. \end{cases} \tag{8}$$

Further restrictions on r may be obtained from the system of equations a lemmas 5,7. If these restrictions turn out to be contradictory no stabl operator with maximal order exists. Otherwise we compute the determinan of the system and obtain a polynomial of degree $k' + k$ but has P^k_{k+1} or $\bar{P}$ a factor. Thus an algebraic equation of degree k-1 has finally to be solved to find a value of r which, hopefully, satisfies all the restrictions.

The following lemma will simplify the construction of optimal stable methods.

<u>Lemma 7</u> The polynomial $P^k_{k+j}(r)$ can be written in the form

$$P^k_{k+j}(r) = \sum_{i=1}^{j} 2^i \binom{j-1}{j-i} \binom{r}{k+i}. \tag{9}$$

<u>Proof</u>:

$$\sum_{j=0}^{\infty} D_j z^j = \frac{\left(\frac{1-z}{2}\right)^k \rho\left(\frac{1+z}{1-z}\right)}{\left(\log\left(\frac{1+z}{1-z}\right)\right)^2} = \left(\frac{1-z}{2}\right)^k \sum_{j=0}^{\infty} d_j \left(\frac{1+z}{1-z} - 1\right)^j$$

$$= \sum_{j=0}^{\infty} d_j 2^{j-k} z^j (1-z)^{k-j}.$$

Thus

$$D_{k+i} = \sum_{j=1}^{i} d_{k+j}\, 2^j (-1)^{i-j} \binom{-j}{i-j} = \sum_{j=1}^{i} d_{k+j}\, 2^j \binom{i-1}{i-j}. \tag{10}$$

Combine (10) with lemmas 2 and 3 yields (9). (9) is particularly helpful for the evaluation of the quotients

$$Q_\ell{}^k(r) := \frac{P^k_{k+2\ell+1}(r)}{P^k_{k+1}} \tag{11}$$

and

$$\tilde{Q}^k_\ell(r) := \frac{P^k_{k+2\ell+2}(r)}{P^k_{k+2}(r)}. \tag{12}$$

<u>Examples</u>

I. k=3, k'=2

Find A_2, A_3, β_r such that

$$\beta_r P_4^3(r) = \Gamma_4' A_2$$

$$\beta_r P_5^3(r) = \Gamma_4' A_3 \tag{13}$$

$$\beta_r \binom{r}{k} = (\Gamma_0' + \Gamma_2') A_2 + (\Gamma_0' + \Gamma_2') A_3$$

A_2 will be taken to be 1.

It can be shown that

$$r^2-2r-3-5 \frac{\Gamma_4'}{\Gamma_0'+\Gamma_2'} = 0. \tag{14}$$

The only acceptable root is r = 2.7320522.

For this r one obtains

$$\beta_r = .215469$$

$$A_3 = .4928203$$

The coefficients α_j, β_j are given by

$\alpha_0 = 2.9433755$, $\alpha_1 = -4.886751$, $\alpha_2 = .9433754$, $\alpha_3 = 1$,

$\beta_0 = .0173967$, $\beta_1 = 1.542232$, $\beta_2 = 2.1411683$.

The following method of order 6 is then obtained

$$y_{n+3} + .9433754\, y_{n+2} - 4.886751\, y_{n+1} + 2.943375\, y_n =$$

$$h^2(.0173967\, f_n + 1.5422232\, f_{n+1} + 2.1411683\, f_{n+2} \tag{15}$$

$$+ .215469\, f_{n+2.732052})$$

II. k=k'=4

Find A_2, A_3, A_4, β_r such that

$$
\begin{aligned}
&\text{(i)} \quad \beta_r P_5^4(r) = D_5 = \Gamma_4' A_3 \\
&\text{(ii)} \quad \beta_r P_6^4(r) = D_6 = \Gamma_4' A_4 + \Gamma_6' A_2 \\
&\text{(iii)} \quad \beta_r P_7^4(r) = D_7 = \Gamma_6' A_3 \\
&\text{(iv)} \quad \beta_r P_8^4(r) = D_8 = \Gamma_6' A_4 + \Gamma_8' A_2
\end{aligned} \tag{16}
$$

A_2 will be taken to be 1.

From (iii)/(i) we have

$$\frac{(2r-4)^2+6}{42} = Q_1^4(r) = \frac{P_7^4(r)}{P_5^4(r)} = \frac{\Gamma_6'}{\Gamma_4'} = .5079364$$

$$
\begin{aligned}
(2r-4)^2 &= 15.\bar{3} \\
2r-4 &= \pm\, 3.91575 \\
r_1 &= 3.957875 \\
r_2 &= .04211
\end{aligned}
$$

It turns out that these are the zeros of the determinant of the system. Note that only r_1 satisfies the stability condition (8). The system can now be solved for the A_i and yields $A_2=1$, $A_3=.793357$, $A_4=.00983138$, $\beta_r=.8580827$. The polynomial $\rho(\zeta)=1.903188\zeta^4 -1.6260388\zeta^3 -1.941022\zeta^2 +1.547388\zeta+ .2164753$.

The coefficients B_i are as follows

$B_0=.1963698$, $B_1=-.0116648$, $B_2=-.4705706$, $B_3=-.318896$, $B_4=-.0490925$.

Thus the second characteristic polynomial

$\sigma(\zeta) = -.758837\zeta^4 +1.596311\zeta^3 +1.824805\zeta^2 +.367384\zeta +.0072672$.

The following method of order 9 is obtained

$$
\begin{aligned}
&y_{n+4} - .8543763\, y_{n+3} - 1.019879\, y_{n+2} + .8130508\, y_{n+1} + .1137435\, y_n \\
&= h^2(.0038184\, f_n + .1930378\, f_{n+1} + .9588148\, f_{n+2} + .8387563\, f_{n+3} \\
&\quad - .3987188\, f_{n+4} + .4508657\, f_{n+3.9578899}).
\end{aligned}
$$

§5. Numerical Experiments

In this section we report on some of the numerical experiments performed. The following two simple differential equations were solved using method (3.35) of order 5 and method (4.15) of order 6.

$$\text{I.}\quad y'' = y \quad 0 < x < 1 \qquad y(0) = 1 \qquad y'(0) = 1 \qquad y_{exact} = e^x \tag{1}$$

$$\text{II.}\quad y'' = -y \quad 0 < x < 2\pi \qquad y(0) = 1 \qquad y'(0) = 0 \qquad y_{exact} = \cos x \tag{2}$$

The predictors used can be obtained (see Lambert [7]) by solving a system of equations.

Predictor for method (3.35):

$$y_{n+2.8} = .8y_{n+2} + 1.2\, y_{n+1} - y_n + h^2\,(.781733\, f_{n+2} + .828533\, f_{n+1} + .109733\, f_n). \tag{3}$$

Predictor for method (4.15):

$$y_{n+3.732052} = -2.778418\, y_{n+3} + 8.123930\, y_{n+2} - 4.180555\, y_{n+1} - .164957\, y_n + h^2(.986623\, f_{n+3} + 3.743048\, f_{n+2} + .585227\, f_{n+1} - .005498\, f_n). \tag{4}$$

The results for various values of n for each problem and method are given in the following four tables. The order of the method was computed numerically and shown to be at least as it was proved theoretically.

n	Error	P
10	.54982119(-5)	4.69
20	.16540029(-6)	4.84
30	.21363790(-7)	4.89
40	.50158089(-8)	4.92
50	.16325752(-8)	4.93
60	.65308425(-9)	4.94
70	.30115020(-9)	4.95
80	.15407098(-9)	4.96
90	.85328238(-10)	

Table I

Problem (I), method (3.35) of order 5

n	Error	P
10	.55863299(-7)	5.56
20	.87891486(-9)	5.80
30	.75632642(-9)	5.87
40	.13281541(-10)	5.90
50	.34502395(-11)	5.92
60	.11480433(-11)	5.94
70	.45309596(-12)	5.95
80	.20239435(-12)	5.95
90	.99639686(-13)	

Table II

Problem (I), method (4.15) of order 6

n	Error	P
10	.12554858(-2)	
20	.33795300(-4)	4.84
30	.41327168(-5)	4.97
40	.94311463(-6)	4.99
50	.30172961(-6)	4.99
60	.11931829(-6)	4.99
70	.54567916(-7)	5.00
80	.27744983(-7)	5.00
90	.15291934(-7)	5.00

Table III

Problem (II), method (3.35) of order 5

n	Error	P
10	.24116254(-4)	
20	.45827052(-7)	8.38
30	.23188211(-8)	7.06
40	.30586932(-9)	6.84
50	.64652911(-10)	6.81
60	.62572205(-11)	6.82
70	.24776324(-11)	6.84
80	.10940173(-11)	6.86

Table IV

Problem (II), method (4.15) of order 6.

Note the superconvergence in this last experiment.

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