

TR/02/81

April 1981

One step multiderivative methods  
for first order  
ordinary differential equations.

E. H. Twizell  
and  
A.Q.M. Khaliq

(0)

0. Abstract

A family of one-step multiderivative methods based on Padé approximants to the exponential function is developed.

The methods are extrapolated and analysed for use in *PECE* mode.

Error constants and stability intervals are calculated and the combinations compared with well known linear multi-step combinations and combinations using high accuracy Newton-Cotes quadrature formulas as correctors.

(1)

## 1. Introduction

Consider a real first order system of ordinary differential equations of order  $N$  given by

$$(0) \quad \underline{y}'(x) = \underline{f}(x, \underline{y}), \quad \underline{y} \in E^N$$

for which all solutions are assumed to be bounded. In the particular case of the linear initial value problem

$$(1) \quad \underline{y}'(x) = A \underline{y}(x), \quad \underline{y}(x_0) = \underline{y}_0,$$

where  $A$  is a square matrix of order  $N$  with constant coefficients, this means that the real parts of the eigenvalues of  $A$  must be non—positive. It is therefore appropriate to consider the test equation

$$(2) \quad y' = \lambda y \quad (\lambda < 0), \quad y(x_0) = y_0$$

and to seek, the solution in some interval  $x_0 = a \leq x \leq b$ . In the case of a single equation of the form (0),  $\lambda$  takes the value of  $\partial f/\partial y$ , estimated at each step.

A family of one-step multiderivative methods based on Padé approximants to the exponential function will be developed. Multiderivative methods are known to give high accuracy when used to solve problems for which higher derivatives are available (see, for example, Lambert [3 ; p.202]). The principal part of the truncation error will be given and for the twenty four members of the family quoted, intervals of absolute stability will be given ; a theorem for unconditional stability will be proved. The family will be seen to contain five well known methods.

In Section 4 the methods will be extrapolated to achieve higher accuracy and in Section 5 the methods will be employed in appropriate predictor-corrector pairs. Intervals of absolute stability, which are seen to be small, are given for *PECE* mode.

(2)

The application of the methods to the heat equation and to first order hyperbolic equations will be considered in two future papers, Multiderivative methods for second order equations will also be considered in a future paper.

(3)

## 2. Derivation of the formulas

Suppose the independent variable  $x$  is incremented using a constant step size  $h = (b - a)/N$  where  $N$  is a positive integer, then the solution of equation (2) will be computed at the points  $x_i = ih$  ( $i = 1, 2, \dots, N$ ).

It is easy to show that the solution  $y(x)$  satisfies the one-step relation

$$(3) \quad y(x + h) = e^{\lambda h} y(x) .$$

Using this relation, any numerical method will determine the solution  $y_{n+1}$  ( $n = 0, 1, \dots, N-1$ ) whose accuracy will depend on the approximation to  $e^{\lambda h}$  used in (3). Using the  $(m, k)$  Padé approximant to  $e^{\lambda h}$  of the form

$$e^{\lambda h} \simeq R_{m,k}(\lambda h) = P_k(\lambda h)/Q_m(\lambda h) + O(h^{m+k+1}) ,$$

where  $P_k, Q_m$  are polynomials of degree  $k, m$ , respectively, defined by

$$(4) \quad P_k(\theta) = 1 + p_{1,k}\theta + p_{2,k}\theta^2 + \dots + p_{k,k}\theta^k; P_0(\theta) \equiv 1$$

and

$$(5) \quad Q_m(\theta) = 1 - q_{1,m}\theta + q_{2,m}\theta^2 - \dots + (-1)^m q_{m,m}\theta^m; Q_0(\theta) \equiv 1$$

with  $p_{1,k} > p_{2,k} > \dots > p_{k,k} > 0$  and  $q_{1,m} > q_{2,m} > \dots > q_{m,m} > 0$

depending on the chosen Padé approximant, equation (3) takes the form

$$(6) \quad \begin{aligned} & (1 - q_{1,m}\lambda h + q_{2,m}\lambda^2 h^2 + \dots + (-1)^m q_{m,m}\lambda^m h^m)y_{n+1} \\ & = (1 + p_{1,k}\lambda h + p_{2,k}\lambda^2 h^2 + \dots + p_{k,k}\lambda^k h^k)y_n \end{aligned}$$

or

$$(7) \quad \begin{aligned} & y_{n+1} - q_{1,m} h y'_{n+1} + q_{2,m} h^2 y''_{n+1} + \dots + q_{m,m} h^m y_{n+1}^{(m)} \\ & = y_n + p_{1,k} h y'_n + p_{2,k} h^2 y''_n + \dots + p_{k,k} h^k y_n^{(k)} . \end{aligned}$$

(4)

Equation (7) is a one-step multiderivative formula which is explicit if  $m = 0$  (Taylor's series of order  $k$ ) and implicit if  $m \neq 0$ ; it is assumed that  $y(x)$  is sufficiently often differentiable on  $[a,b]$ .

The non-zero coefficients of (7) for the family of algorithms yielded by the first twenty four entries of the Padé Table for the exponential function are given in the Appendix. It is seen that the methods based on the (0,1), (1,1) and (3,3) Padé approximants are respectively the Euler predictor, the Euler corrector or trapezoidal rule and Milne's starting procedure (Milne [7]); the methods based on the (k,k) Padé approximants ( $k \geq 1$ ) are one-step Obrech koff methods and are given for  $k = 2,3,4$  in, for example, Lambert [3 ; p.47] and Lambert and Mitchell [4 : Table I].

### 3. Analyses of the methods

With the multiderivative formula (7) may be associated the linear difference operator  $L$  defined by

$$(8) \quad L[y(x); h] = y(x+h) - y(x) + \sum_{i=1}^m (-1)^m q_{i,m} h^i y^{(i)}(x+h) - \sum_{i=1}^k p_{i,k} h^i y^{(i)}(x).$$

Expanding  $y(x+h)$  and its derivatives as Taylor series about  $x$ , and collecting terms, gives

$$(9) \quad L[y(x);h] = C_0 y(x) + C_1 h y'(x) + \dots + C_t h^t y^{(t)}(x) + \dots$$

where the  $C_t$  are constants. The operator  $L$  and the associated multiderivative method (7) are of order  $s$  if in (9),  $C_0 = C_1 = \dots = C_s = 0$  and  $C_{s+1} \neq 0$ ; the term  $C_{s+1} \dots$  is the principal part of the truncation error, known as the error constant. The error constants for the twenty four methods to be considered are contained in Table I.

The multiderivative formula (2) is said to be consistent with the differential equation if the order  $s \geq 1$ ; the twenty-four methods contained in the appendix are clearly consistent.

Writing (7) in the form

$$(10) \quad y_{n+1} - y_n = \sum_{i=1}^k p_{i,k} h^i y_n^{(i)} + \sum_{j=1}^m (-1)^{j+1} q_{j,m} h^j y_{n+1}^{(j)}$$

it is clear that the multiderivative methods are generated by the characteristic polynomials

$$(11) \quad \rho(r) = r-1, \quad \sigma_{i,k}(r) = p_{i,k}, \quad \gamma_{j,m}(r) = (-1)^{j+1} q_{j,m} r^j$$

( $i = 1, \dots, k$ ;  $j = 1, \dots, m$ ). The polynomial equation  $\rho(r) = 0$  has only one zero,  $r = 1$ , and the twenty four consistent multiderivative methods are therefore zero-stable and thus convergent.

(6)

The interval of absolute stability of equation (7) is determined by computing the interval of values of  $\bar{h} = \lambda h$  for which the zero of the stability equation

$$(12) \quad \pi(r, \bar{h}) = 0$$

is less than unity in modulus, where

$$(13) \quad \begin{aligned} \pi(r, \bar{h}) &= \rho(r) - \sum_{i=1}^k \bar{h}^i \sigma_{i,k}(r) - \sum_{j=1}^m \bar{h}^j \gamma_{j,m}(r), \\ &= (1 + \sum_{j=1}^m (-1)^j q_{j,m} \bar{h}^j) r - (1 + \sum_{i=1}^k p_{i,k} \bar{h}^i), \\ &= Q_m(\bar{h})r - p_k(\bar{h}). \end{aligned}$$

The intervals of absolute stability for the multiderivative methods based on the first twenty-four padé approximants to the exponential function are contained in Table I (the figures containing a decimal point have been truncated with two decimal places).

The formulas based on those  $(m,k)$  Padé approximants for which  $m \geq k$  are seen to be unconditionally stable. This is verified by the following theorem whose proof is based on the properties of the coefficients  $P_{i,k}, q_{j,m}$  ( $i = 1, \dots, k$  ;  $j = 1, \dots, m$ ):

Theorem:

The multiderivative method (7) is absolutely stable if and only if  $m \geq k$ .

Proof:

Assume  $m \geq k$  ; then the coefficients in the  $(m,k)$  padé approximant satisfy  $q_{i,m} \geq p_{i,m} \geq 0$  for all  $i = 1, \dots, m$  ( $m,k$  odd or even).



(7)

The requirement  $|r| < 1$  leads to

$$(14) \quad -1 < \frac{1 + p_{1,k} \bar{h} + p_{2,k} \bar{h}^2 + \dots + p_{k,k} \bar{h}^k}{1 - q_{1,m} \bar{h} + q_{2,m} \bar{h}^2 - \dots + (-1)^m q_{m,m} \bar{h}^m} < 1.$$

The left hand side implies the requirement

$$2 + (p_{1,k} - q_{1,m}) \bar{h} + (p_{1,k} - q_{1,m}) \bar{h}^2 + \dots + (p_{k,k} + (-1)^k q_{k,m}) \bar{h}^k + (-1)^{k+1} q_{k+1,m} \bar{h}^{k+1} + \dots + (-1)^m q_{m,m} \bar{h}^m > 0$$

and, since  $q_{i,m} \geq p_{i,k} \geq 0$  for  $m \geq k$  ( $m, k$  odd or even), this inequality is satisfied for  $\bar{h} < 0$ . The right hand side of (14) implies the requirement

$$(p_{1,k} + q_{1,m}) \bar{h} + (p_{2,k} + q_{2,m}) \bar{h}^2 + \dots + (p_{k,k} - (-1)^k q_{k,m}) \bar{h}^k - (-1)^{k+1} q_{k+1,m} \bar{h}^{k+1} + \dots - (-1)^m q_{m,m} \bar{h}^m < 0$$

and this inequality is also satisfied for  $\bar{h} < 0$ .

The multiderivative method given by (7) is thus absolutely stable if  $m \geq k$ .

If  $m < k$  the method has only a finite interval of absolute stability as illustrated, for example, by the (0,1) method which is the Euler predictor formula.

The hypothesis of the theorem is thus proved (see also [1] and [2]).

The methods based on the (k,k) Padé approximants are optimal in that they have the smallest truncation errors; they are also absolutely stable. When used as correctors in *PECE* mode, however, they give smaller intervals of absolute stability, when used with the (0,ℓ) method as predictor ( $\ell = 1, \dots, k$ ), than the methods with  $m < k$ . This will be dealt with more fully in Section 5.

Table I: Stability intervals and principal error terms of the one-step multiderivative formulas

Method (Padé)	Stability interval	error constant
(0,1)	$\bar{h} \in (-2,0)$	$C_2 = 1/2$
(1,1)	$\bar{h} \in (-\infty,0)$	$C_3 = -1/12$
(1,0)	$\bar{h} \in (-\infty,0)$	$C_2 = -1/2$
(0,2)	$\bar{h} \in (-2,0)$	$C_3 = 1/2$
(1,2)	$\bar{h} \in (-6,0)$	$C_4 = -1/72$
(2,2)	$\bar{h} \in (-\infty,0)$	$C_5 = 1/720$
(2,1)	$\bar{h} \in (-\infty,0)$	$C_4 = 1/72$
(2,0)	$\bar{h} \in (-\infty,0)$	$C_3 = 1/6$
(0,3)	$\bar{h} \in (-2.51,0)$	$C_4 = 1/24$
(1,3)	$\bar{h} \in (-5.41,0)$	$C_5 = -1/480$
(2,3)	$\bar{h} \in (-11.84,0)$	$C_6 = 1/7200$
(3,3)	$\bar{h} \in (-\infty,0)$	$C_7 = -1/100800$
(3,2)	$\bar{h} \in (-\infty,0)$	$C_6 = -1/7200$
(3,1)	$\bar{h} \in (-\infty,0)$	$C_5 = -1/480$
(3,0)	$\bar{h} \in (-\infty,0)$	$C_4 = -1/24$
(0,4)	$\bar{h} \in (-2.78,0)$	$C_5 = 1/120$
(1,4)	$\bar{h} \in (-5.43,0)$	$C_6 = -1/3600$
(2,4)	$\bar{h} \in (-9.64,0)$	$C_7 = 1/75600$
(3,4)	$\bar{h} \in (-19.15,0)$	$C_8 = 1/1411200$
(4,4)	$\bar{h} \in (-\infty,0)$	$C_9 = 1/25401600$
(4,3)	$\bar{h} \in (-\infty,0)$	$C_8 = 1/1411200$
(4,2)	$\bar{h} \in (-\infty,0)$	$C_7 = 1/75600$
(4,1)	$\bar{h} \in (-\infty,0)$	$C_6 = 1/3600$
(4,0)	$\bar{h} \in (-\infty,0)$	$C_5 = 1/120$

#### 4. Extrapolation of the methods

Applying equation (3) over two single intervals  $h$  and replacing  $e^{2\lambda h}$  by, for example, its (1,1) Padé approximant, gives

$$\begin{aligned}
 (15) \quad y(x+2h) &= (1+\frac{1}{2}\lambda h)(1+\frac{1}{2}\lambda h)^{-1}(1+\frac{1}{2}\lambda h)(1+\frac{1}{2}\lambda h)^{-1}y(x) \\
 &= (1+2\lambda h+2\lambda^2 h^2+\frac{3}{2}\lambda^3 h^3+\lambda^4 h^4+\frac{5}{8}\lambda^5 h^5)y(x)+O(h^6) \\
 &= y(x)+2hy'(x)+2h^2y''(x)+\frac{3}{2}h^3y'''(x)+h^4y^{(iv)}(x)+\frac{5}{8}h^5y^{(v)}(x)+O(h^6).
 \end{aligned}$$

Alternatively if equation (3) is written over a double interval  $2h$ ,  $y(x+2h)$  is given by

$$\begin{aligned}
 (16) \quad y(x+2h) &= (1+\lambda h)(1-\lambda h)^{-1}y(x) \\
 &= (1+2\lambda h+2\lambda^2 h^2+2\lambda^3 h^3+2\lambda^4 h^4+2\lambda^5 h^5)y(x)+O(h^6) \\
 &= y(x)+2hy'(x)+2h^2y''(x)+2h^3y'''(x)+2h^4y^{(iv)}(x)+2h^5y^{(v)}(x)+O(h^6).
 \end{aligned}$$

The Maclaurin expansion of  $y(x+2h)$  about  $x$  produces

$$\begin{aligned}
 (17) \quad y(x+2h) &= y(x)+2hy'(x)+2h^2y''(x)+\frac{4}{3}h^3y'''(x)+\frac{2}{3}h^4y^{(iv)}(x)+\frac{4}{15}h^5y^{(v)}(x) \\
 &\quad +\frac{4}{45}h^6y^{(vi)}(x)+\frac{8}{315}h^7y^{(vii)}(x)+\frac{2}{315}h^8y^{(viii)}(x)+\frac{4}{2835}h^9y^{(ix)}(x)+O(h^{10}),
 \end{aligned}$$

and defining the values of  $y(x+2h)$  yielded by (15) and (16) to be  $y_{n+2}^{(1)}$

and  $y_{n+2}^{(2)}$  respectively .it is seen that neither is  $O(h^3)$  accurate.

However, defining  $y_{n+2}^{(E)}$  by

$$y_{n+2}^{(E)} = \frac{4}{3}y_{n+2}^{(1)} - \frac{1}{3}y_{n+2}^{(2)}$$

gives

$$(18) \quad y_{n+2}^{(E)} = y(x) + 2hy'(x) + 2h^2y''(x) + \frac{4}{3}h^3y'''(x) + \frac{2}{3}h^4y^{(iv)}(x) + O(h^5)$$

The error in  $y_{n+2}^{(E)}$ , defined by  $y(x+2h) - y_{n+2}^{(E)}$  has principal part  $E_5 = \frac{1}{10}$ .

The second order method based on the (1,1) Padé approximant has been extrapolated to give fourth order accuracy (see also Lindberg [6]) by the Richardson technique.

(10)

Repeating the process for the (3,3) Padé method (Milne's method [7]) leads to

$$\begin{aligned} y_{n+1}^{(1)} &\equiv \left[ \left( 1 + \frac{1}{2}\lambda h + \frac{1}{10}\lambda^2 h^2 + \frac{1}{120}\lambda^3 h^3 \right) \left( 1 - \frac{1}{2}\lambda h + \frac{1}{10}\lambda^2 h^2 - \frac{1}{120}\lambda^3 h^3 \right)^{-1} \right]^2 y(x) \\ &= y(x) + 2hy'(x) + 2h^2 y''(x) + \frac{4}{3}h^3 y'''(x) + \frac{2}{3}h^4 y^{(iv)}(x) + \frac{4}{15}h^5 y^{(v)}(x) \\ &\quad + \frac{4}{45}h^6 y^{(vi)}(x) + \frac{61}{2400}h^7 y^{(vii)}(x) + \frac{23}{3600}h^8 y^{(viii)}(x) + \frac{209}{144000}h^9 y^{(ix)}(x) + 0(h^{10}). \end{aligned}$$

and

$$\begin{aligned} y_{n+1}^{(2)} &\equiv \left( 1 + \lambda h + \frac{2}{5}\lambda^2 h^2 + \frac{1}{15}\lambda^3 h^3 \right) \left( 1 - \lambda h + \frac{2}{5}\lambda^2 h^2 - \frac{1}{15}\lambda^3 h^3 \right) y(x) \\ &= y(x) + 2hy'(x) + 2h^2 y''(x) + \frac{4}{3}h^3 y'''(x) + \frac{2}{3}h^4 y^{(iv)}(x) + \frac{4}{15}h^5 y^{(v)}(x) \\ &\quad + \frac{4}{45}h^6 y^{(vi)}(x) + \frac{2}{75}h^7 y^{(vii)}(x) + \frac{2}{225}h^8 y^{(viii)}(x) + \frac{14}{3375}h^9 y^{(ix)}(x) + 0(h^{10}). \end{aligned}$$

Defining  $y_{n+2}^{(E)}$ , in this case, by

$$(19) \quad y_{n+2}^{(E)} = \frac{64}{63}y_{n+2}^{(1)} - \frac{1}{63}y_{n+2}^{(2)}$$

gives

$$\begin{aligned} y_{n+2}^{(E)} &= y(x) + 2hy'(x) + 2h^2 y''(x) + \frac{4}{3}h^3 y'''(x) + \frac{2}{3}h^4 y^{(iv)}(x) + \frac{4}{15}h^5 y^{(v)}(x) \\ &\quad + \frac{4}{45}h^6 y^{(vi)}(x) + \frac{8}{315}h^7 y^{(vii)}(x) + \frac{2}{315}h^8 y^{(viii)}(x) + \frac{599}{425250}h^9 y^{(ix)}(x) + 0(h^{10}), \end{aligned}$$

which, on comparison with equation (17), is seen to be eighth order

accurate with  $E_9 = \frac{1}{425250}$ . It is clear that as  $m$  and  $k$  increase, the

algebraic manipulation involved in the extrapolation procedure becomes tedious and difficult.

In the cases of the methods based on the (1,1) and (3,3) Padé approximants the extrapolation procedure has produced two extra orders of accuracy.

This phenomenon is a useful feature of multiderivative methods based on (m,m) Padé approximants, which is not evident in methods based on (m,k) Padé approximants ( $m \neq k$ ) for which only a single extra order of accuracy is produced.

(11)

The extrapolating formulas connecting  $y_{n+2}^{(E)}$ ,  $y_{n+2}^{(1)}$  and  $y_{n+2}^{(2)}$  satisfy one

Of the relations

$$(20) \quad y_{n+2}^{(E)} = (2^{m+k} y_{n+2}^{(1)} - y_{n+2}^{(2)}) / (2^{m+k} - 1) + O(h^{m+k+2})$$

when  $m \neq k$ , or

$$(21) \quad y_{n+2}^{(E)} = (2^{2m} y_{n+2}^{(1)} - y_{n+2}^{(2)}) / (2^{2m} - 1) + O(h^{2m+3})$$

when  $m = k$ . The extrapolation formulas for the twenty-four multiderivative methods outlined in Section 2, together with the error constants, the principal parts of their local truncation errors, defined for each method by

$$(22) \quad y(x + 2h) - y_{n+2}^{(E)},$$

are contained in Table II.

It is easy to see that  $y_{n+2}^{(E)}$  may also be written in the form

$$(23) \quad y_{n+2}^{(E)} = \frac{1}{2^{m+k} - 1} \left[ 2^{m+k} \left( \frac{P_k(\lambda h)}{Q_m(\lambda h)} \right)^2 - \frac{P_k(2\lambda h)}{Q_m(2\lambda h)} \right] y_n + O(h^{m+k+2}); m \neq k$$

or

$$(24) \quad y_{n+2}^{(E)} = \frac{1}{2^{2m} - 1} \left[ 2^{2m} \left( \frac{P_m(\lambda h)}{P_m(-\lambda h)} \right)^2 - \frac{P_m(2\lambda h)}{P_m(-2\lambda h)} \right] y_n + O(h^{2m+3}); m = k.$$

Each of (23) and (24) is of the approximate form

$$y_{n+2}^{(E)} \simeq R y_n$$

and clearly the interval of absolute stability for each multiderivative method is the range of values of  $\bar{h} = \lambda h$  for which

$$(25) \quad |R| < 1.$$

The intervals of absolute stability for equations (20) and (21), the extrapolated forms of equation (7), are thus determined by finding the range of values of  $\bar{h}$  for which

(12)

$$(26) \quad (-2^{m+k}+1)[Q_m(\bar{h})]^2 Q_m(2\bar{h}) < 2^{m+k}[P_k(\bar{h})]^2 Q_m(2\bar{h}) - P_k(2\bar{h})[Q_m(\bar{h})]^2 \\ < (2^{m+k}-1)Q_m(\bar{h})]^2 Q_m(2\bar{h})$$

when  $m \neq k$ , or

$$(27) \quad (-2^{2m}+1)[P_m(-\bar{h})]^2 P_m(-2\bar{h}) < 2^{2m}[P_m(\bar{h})]^2 P_m(-2\bar{h}) - P_m(2\bar{h})[P_m(-\bar{h})]^2 \\ < (2^{2m}-1)[P_m(-\bar{h})]^2 P_m(-2\bar{h})$$

when  $m = k$ ,

Thus, for example, the interval of absolute stability for the extrapolated form of the method based on the (1,1) Padé approximant, is the interval of values of  $\bar{h}$  for which

$$(28) \quad -12 + 24\bar{h} - 15\bar{h}^2 + 3\bar{h}^3 < 12 - 9\bar{h}^2 - 5\bar{h}^3 < 12 - 24\bar{h} + 15\bar{h}^2 - 3\bar{h}^3,$$

where fractions have been cleared. The left hand side of (28) is satisfied for all  $\bar{h} < 0$  while the right hand side is satisfied only for the interval  $\bar{h} \in (-11.53, 0)$ , which is therefore the interval of absolute stability.

Clearly, as  $m$  and  $k$  increase, the algebraic manipulation involved in solving (26) or (27) becomes complicated. The interval of absolute stability of the extrapolated form of the multiderivative method based on the (3,3) padé approximant, for example, is found by solving the inequality

$$(29) \quad -13608000 + 27216000\bar{h} - 25174800\bar{h}^2 + 14061600\bar{h}^3 - 5193720\bar{h}^4 \\ + 1315440\bar{h}^5 - 229257\bar{h}^6 + 26649\bar{h}^7 - 1840\bar{h}^8 + 63\bar{h}^9 \\ < 13608000 - 2041200\bar{h}^2 + 204120\bar{h}^4 - 27783\bar{h}^6 - 8775\bar{h}^7 \\ - 1134\bar{h}^8 - 65\bar{h}^9 \\ < 13608000 - 27216000\bar{h} + 25174800\bar{h}^2 - 14061600\bar{h}^3 + 5193720\bar{h}^4 \\ - 1315440\bar{h}^5 + 229257\bar{h}^6 - 26649\bar{h}^7 + 1840\bar{h}^8 - 63\bar{h}^9,$$

(13)

where, again, fractions have been cleared. Both sides of (29) are satisfied for all  $\bar{h} < 0$  and the interval of absolute stability is therefore  $\bar{h} \in (-\infty, 0)$ .

The intervals of absolute stability for the extrapolated forms of all twenty four multiderivative methods derived in Section 2 are also contained in Table II. It must be noted that, whilst extrapolation has improved accuracy, this has often been at the expense of a decreased interval of absolute stability. This is particularly so with the (0,1) and (1,1) Padé methods which are, of course, the Euler predictor formula and the Euler corrector formula (the trapezoidal rule) respectively. The extrapolated form of the (1,1) method does not satisfy Theorem 1 which, therefore, does not hold for the extrapolation formulas.

The extrapolated forms of the twenty four multiderivative methods were tested on the initial value problem

$$y' = -y \quad ; \quad y(0) = 1.$$

In each case were  $y_{n+2}^{(1)}$  and  $y_{n+2}^{(2)}$  computed from the appropriate binomial expansions of the forms (15) and (16) and  $y_{n+2}^{(E)}$  was then computed from the appropriate extrapolation formula (20) or (21) ; the error was calculated from the relevant equation of the form (22). The numerical results for the multiderivative methods, before extrapolation, were computed from the appropriate equations of the form (6) and the errors calculated from (22).

The step size  $h$  was given the values 0.05, 0.1, 0.2 and the errors for all methods were found to be as indicated in the theory. The numerical results at  $x = 0.4, 0.8$  for the methods based on the (1,1) and (3,3) Padé approximants, whose error constants and stability intervals in

(14)

extrapolated form have been considered in detail above, are given in Table III to two significant figures.



Table II : The extrapolating algorithms

Method (Padé)	Extrapolating algorithm	Stability interval	error constant
(0,1)	$2y^{(1)}-y^{(2)}$	$\bar{h} \in (-1,0)$	$E_3 = \frac{4}{3}$
(1,1)	$(4y^{(1)}-y^{(2)})/3$	$\bar{h} \in (-11.53,0)$	$E_5 = \frac{1}{10}$
(1,0)	$2y^{(1)}-y^{(2)}$	$\bar{h} \in (-\infty,0)$	$E_3 = \frac{4}{3}$
(0,2)	$(4y^{(1)}-y^{(2)})/3$	$\bar{h} \in (-2.57,0)$	$E_4 = -\frac{1}{3}$
(1,2)	$(8y^{(1)}-y^{(2)})/7$	$\bar{h} \in (-6.47,0)$	$E_5 = -\frac{8}{945}$
(2,2)	$(16y^{(1)}-y^{(2)})/15$	$\bar{h} \in (-\infty,0)$	$E_7 = -\frac{1}{1890}$
(2,1)	$(8y^{(1)}-y^{(2)})/7$	$\bar{h} \in (-\infty,0)$	$E_5 = -\frac{8}{945}$
(2,0)	$(4y^{(1)}-y^{(2)})/3$	$\bar{h} \in (-\infty,0)$	$E_4 = -\frac{1}{3}$
(0,3)	$(8y^{(1)}-y^{(2)})/7$	$\bar{h} \in (-2.02,0)$	$E_5 = \frac{8}{105}$
(1,3)	$(16y^{(1)}-y^{(2)})/15$	$\bar{h} \in (-6.20,0)$	$E_6 = -\frac{1}{540}$
(2,3)	$(32y^{(1)}-y^{(2)})/31$	$\bar{h} \in (-11.44,0)$	$E_7 = \frac{4}{5425}$
(3,3)	$(64y^{(1)}-y^{(2)})/63$	$\bar{h} \in (-\infty,0)$	$E_9 = \frac{1}{425250}$
(3,2)	$(32y^{(1)}-y^{(2)})/31$	$\bar{h} \in (-\infty,0)$	$E_7 = \frac{4}{5425}$
(3,1)	$(16y^{(1)}-y^{(2)})/15$	$\bar{h} \in (-\infty,0)$	$E_6 = \frac{1}{540}$
(3,0)	$(8y^{(1)}-y^{(2)})/7$	$\bar{h} \in (-\infty,0)$	$E_5 = \frac{8}{105}$
(0,4)	$(16y^{(1)}-y^{(2)})/15$	$\bar{h} \in (-3.23,0)$	$E_6 = \frac{2}{135}$
(1,4)	$(32y^{(1)}-y^{(2)})/31$	$\bar{h} \in (-12.30,0)$	$E_7 = \frac{8}{27125}$
(2,4)	$(64y^{(1)}-y^{(2)})/63$	$\bar{h} \in (-9.62,0)$	$E_8 = -\frac{1079}{127575}$
(3,4)	$(128y^{(1)}-y^{(2)})/127$	$\bar{h} \in (-7.98,0)$	$E_9 = \frac{93341}{88211025}$
(4,4)	$(256y^{(1)}-y^{(2)})/255$	$\bar{h} \in (-\infty,0)$	$E_{11} = -\frac{1}{144317250}$
(4,3)	$(128y^{(1)}-y^{(2)})/127$	$\bar{h} \in (-\infty,0)$	$E_9 = \frac{93341}{88211025}$
(4,2)	$(64y^{(1)}-y^{(2)})/63$	$\bar{h} \in (-\infty,0)$	$E_8 = \frac{1079}{127575}$
(4,1)	$(32y^{(1)}-y^{(2)})/31$	$\bar{h} \in (-\infty,0)$	$E_7 = \frac{8}{27125}$
(4,0)	$(16y^{(1)}-y^{(2)})/15$	$\bar{h} \in (-\infty,0)$	$E_6 = -\frac{2}{135}$

Table III : Error moduli at  $x = 0.4, 0.8$  with  $h = 0.05, 0.1, 0.2$ , for the initial value problem  $y' = y$  ;  $y(0) = 1$  using the methods based on the (1,1) and (3,3) Padé approximants and their extrapolated forms.

x	0.4			0.8		
h	0.05	0.1	0.2	0.05	0.1	0.2
Method	Error moduli			Error moduli		
(1,1) Extrapolated (1,1)	0.60(-4)	0.26(-3)	0.12(-2)	0.81(-4)	0.35(-3)	0.16(-2)
	0.73(-7)	0.15(-5)	0.27(-4)	0.10(-6)	0.20(-5)	0.36(-4)
(3,3) Extrapolated (3,3)	0.28(-7)	0.92(-8)	0.13(-7)	0.48(-7)	0.12(-7)	0.22(-7)
	0.99(-9)	0.10(-9)	0.17(-8)	0.13(-8)	0.13(-8)	0.70(-9)

Theoretical solutions :  $y(0.4) \simeq 0.67$  ,  $y(0.8) \simeq 0.45$ .

### 5. Use in PECE mode

In this section the  $(0,1)$ ,  $(0,2)$ ,  $(0,3)$ ,  $(0,4)$  explicit formulas will be used as predictor formulas and all appropriate combinations of these four formulas with the twenty implicit formulas of Section 2 as correctors will be considered. Predictor-corrector methods for which the order of the predictor exceeds that of the corrector will not be constructed.

Using the general  $(0,k^*)$  Padé approximant as predictor, the characteristic polynomials (from (11)) are

$$(30) \quad \rho^*(r) = r - 1 \quad , \quad \sigma_{i,k^*}^*(r) = p_{i,k^*}$$

where the convention of associating an asterisk with the predictor has been adopted. Using the  $(m,k)$  Padé approximant ( $m \neq 0$ ) as corrector, the characteristic polynomials (11) become

$$P(r) = r - 1 \quad , \quad \sigma_{i,k} (r) = p_{i,k} \quad , \quad (i=1, \dots, k) \quad , \quad \gamma_{j,m} (r) = (-1)^{j+1} q_{j,m} \quad r \quad (j=1, \dots, m).$$

This combination of predictor and corrector will be denoted by  $(0,k^*);(m,k)$ .

The stability polynomial for the  $(0,k^*) ; (m,k)$  predictor-corrector combination in PECE mode is therefore

$$(31) \quad \begin{aligned} \pi_{\text{PECE}} (r, \bar{h}) &= \rho^*(r) - \sum_{i=1}^k \bar{h}^{-i} \sigma_{i,k} (r) - \sum_{j=1}^m \bar{h}^{-j} \gamma_{j,m} (r) \\ &\quad + \sum_{j=1}^m \bar{h}^{-j} \gamma_{j,m} (r) \left[ \rho^* - \sum_{i=1}^{k^*} \bar{h}^{-i} \sigma_{i,k^*}^*(r) \right] \\ &= r - 1 - \sum_{i=1}^k p_{i,k} \\ &\quad + \sum_{j=1}^m (-1)^j q_{j,m} \bar{h}^{-j} \left[ 1 + \sum_{i=1}^{k^*} p_{i,k^*} \bar{h}^{-i} \right] \end{aligned}$$

(18)

and the interval of absolute stability is the range of values of  $h$  for which the zero  $r$  of

$$(32) \quad \pi_{PECE}(r, \bar{h}) = 0$$

is less than unity in modulus.

Solving equation (32) for  $r$  gives

$$(33) \quad r = e^{\bar{h}} - T_{s+1} \bar{h}^{-s+1} + O(\bar{h}^{-s+2})$$

where  $s$  is the order of the predictor-corrector combination  $(0, k^*)$  ;  $(m, k)$ . The term  $T_{s+1}$  is the error constant of the predictor-corrector combination.

The intervals of absolute stability and the error constants are contained in Tables IV, V, VI, and VII for the predictor-corrector combinations using, respectively, the  $(0,1)$ ,  $(0,2)$ ,  $(0,3)$ ,  $(0,4)$  Padé methods as predictors. All possible combinations of these explicit predictors with the other twenty implicit methods used as correctors, for which the order of the predictor does not exceed that of the corrector, are included in the tables.

It is easy to see that for all four predictors, using the  $(1,4)$  method as corrector gives the greatest interval of absolute stability as well as the smallest error modulus ; in the case of the  $(0,3)$  ;  $(1,3)$  combination, one derivative fewer is required in the corrector than in the  $(0,3)$  ;  $(1,4)$  combination for the same accuracy and the same interval of absolute stability.

For all four  $(0, k)$  predictors.  $k = 1, 2, 3, 4$ , it is seen that the  $(0, k)$  ;  $(k, 0)$  predictor-corrector combination gives the worst error in *PECE* mode and the smallest interval of absolute stability, except that the  $(0, 2)$  ;  $(4, 0)$  combination has a slightly smaller stability interval than the  $(0, 2)$ ;  $(2, 0)$  combination. This latter combination does, however, have

a better principal error term and requires lower order derivatives.

The literature contains little on the size of stability intervals for one-step multiderivative methods used in PECE mode. They have been verified in this paper to be generally small, and examination of Tables IV, V, VI, VII shows surprisingly that the greatest stability intervals in PECE mode arise with correctors based on (1,k) formulas which themselves have poor stability intervals (Table I). It can be deduced from Tables IV, V, VI, VII that as (m,k) correctors ( $m = 1, \dots, k$ ), with increasing individual stability intervals, are used with a given predictor, the stability intervals in PECE mode decrease. It can also be deduced that the absolutely stable implicit methods of Section 2 have inferior intervals of stability to those methods with finite stability intervals when used as correctors with any given (0,k) predictor.

Comparisons with the Milne-Simpson and Adams-Bashforth-Moulton combinations show that the results of this section can give much bigger stability intervals than multi-step methods with the same order of accuracy.

Comparisons with the results of Lawson and Ehle [5] show that one-step multiderivative methods can also give comparable accuracy to that of one-step methods which use high accuracy Newton-Cotes quadrature formulas as correctors, but can simultaneously give bigger stability intervals. The use of a combination such as (0,4) ; (1,5) for instance, would give the same overall accuracy as the method of Lawson and Ehle [5] but would have a stability interval bigger than  $\bar{h} \in (-3.21, 0)$ , the stability interval for the (0,4) ; (1,4) combination which has accuracy one power fewer than the method of Lawson and Ehle [5]; the method of Lawson and Ehle [5] has stability interval  $\bar{h} \in (-2.07, 0)$ .

The multiderivate methods in PECE mode were tested on the initial value problem

$$y' = -y ; y(0) = 1.$$

(20)

The step size  $h$  was given the values 0.5, 1.0, 2.0, 3.0, and the solution computed at  $x = 0.0(h)6.0$ . The numerical results obtained conformed fully to the indications of the theory ; that is, as  $h$  increased and  $\bar{h}$  went outside the interval of absolute stability, the error moduli grew quickly and soon swamped the theoretical solution. It is noted that, for the (0,4) ; (4,0) combination, whose stability interval  $\bar{h} \in (-2,0)$  requires  $h$  to be in the interval  $0 < h < 2.0$ , the error modulus for  $h = 20$  falls initially and then begins to rise as  $x$  increases.

The numerical results for the (0,k) ; (k,0) and (0,k) ; (1,4) combinations ( $k = 1,2,3,4$ ), which, for each predictor give the poorest and best results from the points of view of accuracy and stability interval, are given in Table VIII.

(21)

Table IV : Intervals of absolute stability and principal error terms of the correctors used with the  $(0_t 1)$  predictor.

Corrector	Stability interval	error constant
(1,1)	$\bar{h} \in (-2,0)$	$T_3 = 1/6$
(1,0)	$\bar{h} \in (-1,0)$	$T_3 = -1/2$
(1,2)	$\bar{h} \in (-2,0)$	$T_3 = 1/6$
(2,2)	$\bar{h} \in (-1.58,0)$	$T_3 = 1/4$
(2,1)	$\bar{h} \in (-1.37,0)$	$T_3 = 1/3$
(2,0)	$\bar{h} \in (-1,0)$	$T_3 = 2/3$
(1,3)	$\bar{h} \in (-2.53,0)$	$T_3 = 1/8$
(2,3)	$\bar{h} \in (-1.78,0)$	$T_3 = 1/5$
(3,3)	$\bar{h} \in (-1.54,0)$	$T_3 = 1/4$
(3,2)	$\bar{h} \in (-1.39,0)$	$T_3 = 3/10$
(3,1)	$\bar{h} \in (-1.22,0)$	$T_3 = 3/8$
(3,0)	$\bar{h} \in (-1.00,0)$	$T_3 = 1/2$
(1,4)	$\bar{h} \in (-2.61,0)$	$T_3 = 1/10$
(2,4)	$\bar{h} \in (-2.02,0)$	$T_3 = 1/6$
(3,4)	$\bar{h} \in (-1.67,0)$	$T_3 = 3/14$
(4,4)	$\bar{h} \in (-1.52,0)$	$T_3 = 1/4$
(4,3)	$\bar{h} \in (-1.41,0)$	$T_3 = 2/7$
(4,2)	$\bar{h} \in (-1.29,0)$	$T_3 = 1/3$
(4,1)	$\bar{h} \in (-1.16,0)$	$T_3 = 4/5$
(4,0)	$\bar{h} \in (-1.00,0)$	$T_3 = 1/2$

(22)

Table V : Intervals of absolute stability and principal error terms of the correctors used with the(0.2)predictor

Corrector	stability interval	error constant
(1,1)	$\bar{h} \in (-2.0)$	$T_3 = -1/12$
(1,2)	$\bar{h} \in (-2.51,0)$	$T_4 = 1/24$
(2,2)	$\bar{h} \in (-2,0)$	$T_4 = 1/12$
(2,1)	$\bar{h} \in (-1.79,0)$	$T_4 = 1/8$
(2,0)	$\bar{h} \in (-1.61,0)$	$T_3 = 1/6$
(1,3)	$\bar{h} \in (-2.51,0)$	$T_4 = 1/24$
(2,3)	$\bar{h} \in (-2.13,0)$	$T_4 = 1/15$
(3,3)	$\bar{h} \in (-1.94,0)$	$T_4 = 1/12$
(3,2)	$\bar{h} \in (-1.82,0)$	$T_4 = 1/10$
(3,1)	$\bar{h} \in (-1.67,0)$	$T_4 = 1/8$
(3,0)	$\bar{h} \in (-1.50,0)$	$T_4 = 1/8$
(1,4)	$\bar{h} \in (-2.78,0)$	$T_4 = 1/30$
(2,4)	$\bar{h} \in (-2.26,0)$	$T_4 = 1/18$
(3,4)	$\bar{h} \in (-2.05,0)$	$T_4 = 1/14$
(4,4)	$\bar{h} \in (-1.92,0)$	$T_4 = 1/12$
(4,3)	$\bar{h} \in (-1.84,0)$	$T_4 = 2/21$
(4,2)	$\bar{h} \in (-1.74,0)$	$T_4 = 1/9$
(4,1)	$\bar{h} \in (-1.61,0)$	$T_4 = 2/15$
(4,0)	$\bar{h} \in (-1.47,0)$	$T_4 = 1/6$

(23)

Table VI : Intervals of absolute stability and principal error terms of the correctors used with the (0,3) predictor.



Corrector	stability interval	error constant
(1,2)	$\bar{h} \in (-2.38,0)$	$T_4 = -1/72$
(2,2)	$\bar{h} \in (-2.13,0)$	$T_5 = 1/45$
(2,1)	$\bar{h} \in (-2,0)$	$T_4 = 1/72$
(1,3)	$\bar{h} \in (-2.79,0)$	$T_5 = 1/120$
(2,3)	$\bar{h} \in (-2.28,0)$	$T_5 = 1/60$
(3,3)	$\bar{h} \in (-2.09,0)$	$T_5 = 1/48$
(3,2)	$\bar{h} \in (-1.97,0)$	$T_5 = 1/40$
(3,1)	$\bar{h} \in (-1.84,0)$	$T_5 = 7/240$
(3,0)	$\bar{h} \in (-1.59,0)$	$T_4 = 1/8$
(1,4)	$\bar{h} \in (-2.79,0)$	$T_5 = 1/120$
(2,4)	$\bar{h} \in (-2.40,0)$	$T_5 = 1/72$
(3,4)	$\bar{h} \in (-2.19,0)$	$T_5 = 17/1050$
(4,4)	$\bar{h} \in (-2.07,0)$	$T_5 = 1/48$
(4,3)	$\bar{h} \in (-1.99,0)$	$T_5 = 1/42$
(4,2)	$\bar{h} \in (-1.92,0)$	$T_5 = 1/36$
(4,1)	$\bar{h} \in (-1.76,0)$	$T_5 = 1/30$
(4,0)	$\bar{h} \in (-1.59,0)$	$T_5 = 1/12$

(24)

Table VII : Intervals of absolute stability and principal error terms of the correctors used with the (0,4) predictor.

Corrector	Stability interval	error constant
(2,2)	$\bar{h} \in (-2.54,0)$	$T_5 = 1/720$
(1,3)	$h \in (-2.92,0)$	$T_5 = -1/480$
(2,3)	$\bar{h} \in (-2.65,0)$	$T_6 = 1/248$
(3,3)	$\bar{h} \in (-2.48,0)$	$T_6 = 1/240$
(3,2)	$\bar{h} \in (-2.37,0)$	$T_6 = 7/1440$
(3,1)	$\bar{h} \in (-2.21,0)$	$T_5 = -1/480$
(1,4)	$h \in (-3.21,0)$	$T_6 = 1/720$
(2,4)	$\bar{h} \in (-2.76,0)$	$T_6 = 1/360$
(3,4)	$\bar{h} \in (-2.57,0)$	$T_6 = 1/280$
(4,4)	$\bar{h} \in (-2.45,0)$	$T_6 = 1/240$
(4,3)	$\bar{h} \in (-2.37,0)$	$T_6 = 1/80$
(4,2)	$\bar{h} \in (-2.27,0)$	$T_6 = 1/44$
(4,1)	$\bar{h} \in (-2.15,0)$	$T_6 = 1/44$
(4,0)	$\bar{h} \in (-2,0)$	$T_5 = 1/120$

Table VIII: Error moduli at  $x=2.0, 3.0, 4.0, 6.0$  with  $h=0.5, 1.0, 2.0, 3.0$  using the  $(0,k)$  ;  $(k,0)$  and  $(0,k)$  ;  $(1,4)$  predictor-corrector combinations ( $k = 1,2,3,4$ ) to solve the initial value problem  $y' = -y$  ;  $y(0) = 1$ .

			h			
Predictor	Corrector	x	0.5	1.0	2.0	3.0
			Error moduli			
(0,1)	(1,0)	2.0	0.11	0.14	0.29(+1)	-
		3.0	0.75(-1)	0.95	-	0.70(+1)
		4.0	0.44(-1)	0.10(+1)	0.70(+1)	-
		6.0	0.13(-1)	0.30(+1)	0.27(+2)	0.32(+2)
	(1,4)	2.0	0.98(-2)	0.60(-1)	0.46	-
		3.0	0.55(-2)	0.37(-1)	-	0.13(+1)
		4.0	0.27(-2)	0.20(-1)	0.34	-
		6.0	0.58(-3)	0.49(-2)	0.21	0.19(+1)
(0,2)	(2,0)	2.0	0.26(-2)	0.73(-1)	0.31(+1)	-
		3.0	0.14(-2)	0.34(-1)	-	0.18(+2)
		4.0	0.70(-3)	0.14(-1)	0.90(+1)	-
		6.0	0.14(-3)	0.22(-2)	0.27(+2)	0.32(+3)
	(1,4)	2.0	0.16(-2)	0.19(-1)	0.34	-
		3.0	0.90(-3)	0.99(-2)	-	0.14(+1)
		4.0	0.44(-3)	0.47(-2)	0.22(-1)	-
		6.0	0.89(-4)	0.89(-3)	0.10(-1)	0.18(+1)
(0,3)	(3,0)	2.0	0.30(-2)	0.62(-1)	0.26(+1)	-
		3.0	0.16(-2)	0.38(-1)	-	0.25(+2)
		4.0	0.81(-3)	0.21(-1)	0.77(+1)	-
		6.0	0.17(-3)	0.52(-2)	0.21(+2)	0.63(+3)
	(1,4)	2.0	0.21(-3)	0.53(-2)	0.20	-
		3.0	0.12(-3)	0.29(-2)	-	0.13(+1)
		4.0	0.58(-4)	0.15(-2)	0.93(-1)	-
		6.0	0.12(-4)	0.30(-3)	0.35(-1)	0.19(+1)
(0,4)	(4,0)	2.0	0.15(-4)	0.62(-2)	0.11(+1)	-
		3.0	0.81(-5)	0.34(-2)	-	0.20(+2)
		4.0	0.40(-5)	0.16(-2)	0.98	-
		6.0	0.80(-6)	0.32(-3)	0.10(+1)	0.41(+3)
	(1,4)	2.0	0.18(-4)	0.89(-3)	0.69(-1)	-
		3.0	0.10(-4)	0.49(-3)	-	0.70
		4.0	0.49(-5)	0.24(-3)	0.14(-1)	-
		6.0	0.99(-6)	0.49(-4)	0.22(-2)	0.42

x	Theoretical solution
2.0	0.14.
3.0	0.50(-1)
4.0	0.18(-1)
6.0	0.25(-2)

## 6. Summary

A family of linear, one-step, multiderivate methods, based on Padé approximants to the exponential function, has been developed in this paper. The family is seen to contain a number of well known methods including the Euler predictor, the Euler corrector (the trapezoidal rule) and a formula due to Milne [7]. It has been verified that, using comparable steplengths, much higher accuracy can be obtained using the family of one-step multiderivative methods than can be achieved using linear one-step methods. The family of multiderivative methods is therefore appropriate for use in problems which allow higher derivatives to be found explicitly and which require high accuracy. Intervals of absolute stability have been calculated and it is seen that those members of the family which are fully implicit, in the sense that the highest derivative must be evaluated at the advanced point, are absolutely stable.

The family of multiderivative methods is extrapolated to achieve higher accuracy and intervals of absolute stability are calculated for the extrapolation formulas. It is seen that, whilst extrapolation increases accuracy, stability intervals are sometimes shortened as a consequence ; the most notable example of this is the trapezoidal rule.

Finally, the family of one-step multiderivative methods are used in appropriate predictor-corrector pairs. Error constants and stability intervals are calculated for PECE mode. As with linear multistep (single derivative) methods used in PECE mode, the stability intervals are seen to be somewhat low. It is clear from Tables IV, V, VI, VII, however, that it is possible to achieve a bigger stability interval, with comparable accuracy, using one—step multiderivative combinations in PECE mode than with some well known multi-step combinations, notably the

(27)

Milne-Simpson and Adams-Bashforth-Moulton methods, or with one-step methods using high accuracy Newton-Cotes quadrature formulas as correctors.

Appendix: One-step multiderivative methods based on the first twenty-four entries of the Padé Table for the exponential function

- (0,1) :  $y_{n+1} = y_n + hy'_n + O(h^2)$ . (Euler's predictor).
- (1,1) :  $y_{n+1} = y_n + \frac{1}{2}h(y'_n + y'_{n+1}) + O(h^3)$ . (Euler's corrector; the trapezoidal rule).
- (1,0) :  $y_{n+1} = y_n + hy'_{n+1} + O(h^2)$ .
- (0,2) :  $y_{n+1} = y_n + hy'_n + \frac{1}{2}h^2y''_n + O(h^3)$ .
- (0,2) :  $y_{n+1} = y_n + \frac{2}{3}hy'_n + \frac{1}{3}hy'_{n+1} + \frac{1}{6}h^2y''_n + O(h^4)$ .
- (2,2) :  $y_{n+1} = y_n + \frac{1}{2}h(y'_n + y'_{n+1}) + \frac{1}{12}h^2(y''_n - y''_{n+1}) + O(h^5)$ .
- (2,1) :  $y_{n+1} = y_n + \frac{1}{3}hy'_n + \frac{2}{3}hy'_{n+1} - \frac{1}{6}h^2y''_{n+1} + O(h^4)$ .
- (2,0) :  $y_{n+1} = y_n + hy'_{n+1} - \frac{1}{2}h^2y''_{n+1} + O(h^3)$ .
- (0,3) :  $y_{n+1} = y_n + hy'_n + \frac{1}{2}h^2y''_n + \frac{1}{6}h^3y_n^{(iii)} + O(h^4)$ .
- (1,3) :  $y_{n+1} = y_n + \frac{1}{4}h(3y'_n + y'_{n+1}) + \frac{1}{4}h^2y''_n + \frac{1}{24}h^3y_n^{(iii)} + O(h^5)$ .
- (2,3) :  $y_{n+1} = y_n + \frac{1}{5}h(3y'_n + 2y'_{n+1}) + \frac{1}{20}h^2(3y''_n - y''_{n+1}) + \frac{1}{60}h^3y_n^{(iii)} + O(h^6)$ .
- (3,3) :  $y_{n+1} = y_n + \frac{1}{2}h(y'_n + y'_{n+1}) + \frac{1}{10}h^2(y''_n - y''_{n+1}) + \frac{1}{120}h^3(y_n^{(iii)} + y_{n+1}^{(iii)}) + O(h^7)$ . (Milne's starting procedure)
- (3,2) :  $y_{n+1} = y_n + \frac{1}{5}h(3y'_n + 2y'_{n+1}) + \frac{1}{20}h^2(3y''_n - y''_{n+1}) + \frac{1}{60}h^3y_n^{(iii)} + O(h^6)$ .
- (3,1) :  $y_{n+1} = y_n + \frac{1}{4}h(y'_n + 3y'_{n+1}) - \frac{1}{4}h^2y''_{n+1} + \frac{1}{24}h^3y_{n+1}^{(iii)} + O(h^5)$ .
- (3,0) :  $y_{n+1} = y_n + hy'_{n+1} - \frac{1}{2}h^2y''_{n+1} + \frac{1}{6}h^3y_{n+1}^{(iii)} + O(h^4)$ .
- (0,4) :  $y_{n+1} = y_n + hy'_n + \frac{1}{2}h^2y''_n + \frac{1}{6}h^3y_n^{(iii)} + \frac{1}{24}(h^4)y_n^{(iv)} + O(h^5)$
- (1,4) :  $y_{n+1} = y_n + \frac{1}{5}h(4y'_n + y'_{n+1}) + \frac{3}{10}h^2y''_n + \frac{1}{15}h^3y_n^{(iii)} + \frac{1}{120}(h^4)y_n^{(iv)} + O(h^6)$

(29)

$$(2,4) : y_{n+1} = y_n + \frac{1}{3}h(2y'_n + y'_{n+1}) + \frac{1}{5}h^2(y''_n - \frac{1}{6}y''_{n+1}) + \frac{1}{30}h^3 y_n^{(iii)} + \frac{1}{360}h^4 y_n^{(iv)} + 0(h^7).$$

$$(3,4) : y_{n+1} = y_n + \frac{1}{7}h(4y'_n + 3y'_{n+1}) + \frac{1}{14}h^2(2y''_n - y''_{n+1}) + \frac{1}{210}h^3(4y_n^{(iii)} + y_{n+1}^{(iii)}) + \frac{1}{840}h^4 y_n^{(iv)} + 0(h^8).$$

$$(4,4) : y_{n+1} = y_n + \frac{1}{2}h(y'_n + y'_{n+1}) + \frac{3}{28}h^2(2y''_n - y''_{n+1}) + \frac{1}{84}h^3(y_n^{(iii)} + y_{n+1}^{(iii)}) + \frac{1}{1680}h^4(y_n^{(iv)} - y_{n+1}^{(iv)}) + 0(h^9).$$

$$(4,3) : y_{n+1} = y_n + \frac{1}{7}h(y'_n + 4y'_{n+1}) + \frac{1}{14}h^2(y''_n - 2y''_{n+1}) + \frac{1}{210}h^3(y_n^{(iii)} + 4y_{n+1}^{(iii)}) - \frac{1}{840}h^4 y_n^{(iv)} + 0(h^8).$$

$$(4,2) : y_{n+1} = y_n + \frac{1}{3}h(y'_n + 2y'_{n+1}) + \frac{1}{30}h^2(y''_n - 6y''_{n+1}) + \frac{1}{30}h^3 y_{n+1}^{(iii)} - \frac{1}{360}h^4 y_{n+1}^{(iv)} + 0(h^7).$$

$$(4,1) : y_{n+1} = y_n + \frac{1}{5}h(y'_n + 4y'_{n+1}) - \frac{3}{10}h^2 y''_{n+1} + \frac{1}{15}h^3 y_{n+1}^{(iii)} - \frac{1}{120}h^4 y_{n+1}^{(iv)} + 0(h^6).$$

$$(4,0) : y_{n+1} = y_n + hy'_{n+1} - \frac{1}{12}h^2 y''_{n+1} + \frac{1}{6}h^3 y_{n+1}^{(iii)} - \frac{1}{24}h^4 y_{n+1}^{(iv)} + 0(h^5).$$

References

1. 0. Axelsson, "A class of A-stable methods", *BIT*, Vol : 9, 185 - 199, 1969.
2. B.L. Ehle, "High order A-stable methods for the numerical solution of systems of differential equations", *BIT*, Vol : 8, 276 - 278, 1968.
3. J.D. Lambert, *Computational methods in ordinary differential equations*, Wiley, Chichester, 1973.
4. J.D. Lambert and A.R. Mitchell, "On the solution of  $y' = f(x,y)$  by a class of high accuracy difference formulae of low order", *Z. Angew. Math. Phys.*, Vol : 13, 223 - 232, 1962.
5. J.D. Lawson and B.L. Ehle, "Asymptotic error estimation for one-step methods based on quadrature", *Aeq. Math.*, Vol : 5, 236 - 246, 1970.
6. B. Lindberg, "On smoothing and extrapolation for the trapezoidal rule", *BIT*, Vol : 11, 29 - 52, 1971.
7. W.E. Milne, "A note on the numerical integration of differential equations", *J. Res. Nat. Bur. Standards*, Vol : 43, 537 - 542, 1949.

Acknowledgement

The research of one of the authors (AQMK) was partially supported by the Government of Pakistan Merit Scholarship Scheme.

**NOT TO BE  
REMOVED**  
FROM THE LIBRARY

