MATHEMATICS OF COMPUTATION, VOLUME 30, NUMBER 135
JULY 1976, PAGES 417–432

Some New High-Order Multistep Formulae for Solving Stiff Equations

By G. K. Gupta

Abstract. Several new multistep formulae of orders up to 9 for solving stiff ordinary differential equations are presented. Results of numerical testing of these new formulae and some formulae presented in earlier papers and the stiff formulae used by Gear are included.

1. Introduction. In recent papers, Gupta and Wallace (1975) and Wallace and Gupta (1973), the authors have presented several new linear multistep methods (formulae) for the solution of stiff differential equations. In this paper more new multistep formulae are presented. Results of numerical testing of these formulae and those presented in previous papers, using a subroutine similar to DIFSUB of Gear (1971), are included.

We will be using a polynomial representation of the linear multistep methods. Each multistep method of order m can be represented by a corresponding polynomial $C(x)$ of degree m. We have called this the 'modifier polynomial' of the method. This representation was discussed in detail in Wallace and Gupta (1973), where we also show the relation between the coefficients of $C(x)$ and the coefficients $\{\alpha_i\}$ and $\{\beta_i\}$ of the conventional representation of multistep methods.

For each of the formulae we study, we will present its truncation error coefficient K_{m+1} and the stability parameters D and α. The local truncation error introduced in the nth step of numerical integration is given by $K_{m+1}h^{m+1}y^{(m+1)}(x_n) + O(h^{m+2})$ for a method of order m, using a step-size of h (assumed constant). The differential equation being solved is

$$y' = f(x, y), \qquad y(0) = y_0.$$

The stability parameters D and α are defined in the following definition of $A(\alpha, D)$-stability.

Definition. $A(\alpha, D)$-Stability. A method is said to be $A(\alpha, D)$-stable, $\alpha \in (0, \pi/2)$ if all numerical solutions to $y' = \lambda y$ converge to zero as $n \longrightarrow \infty$ with h fixed for all $|\arg(-\lambda h)| < \alpha$, $D \leqslant \mathrm{Re}(h\lambda) < 0$, $|\lambda| \neq 0$ and for all $\mathrm{Re}(h\lambda) \leqslant D$.

$A(\alpha, D)$-stability combines the essential features of the $A(\alpha)$-stability of Widlund (1967) and the stiff-stability of Gear (1969).

Received September 30, 1974; revised March 6, 1975.

AMS (MOS) subject classifications (1970). Primary 65L05; Secondary 65D30.

Key words and phrases. Linear multistep methods, stiff differential equations, numerical solution of ODE.

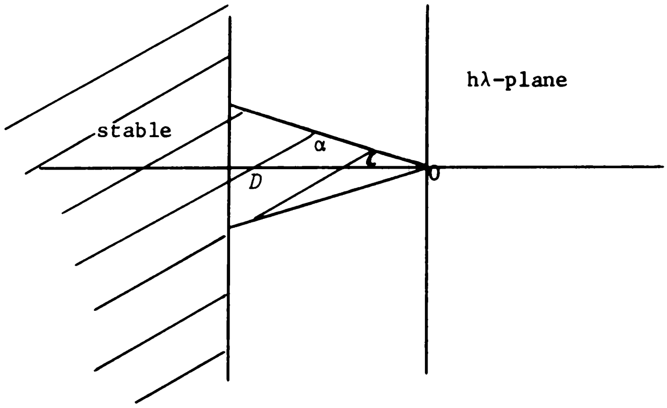

FIGURE 1
The shaded portion is the $A(\alpha, D)$-stability region

2. Formalism. Assuming the step-size to be fixed, as is done in this paper, we define $x_n = nh$ and y_n to be the approximate solution at x_n. Also $f_n = f(x_n, y_n)$.

For an m-step method, we suppose that the solution after the step to x_{n-1} is approximated by a polynomial $P_{n-1}(x)$ of degree m, with $P_{n-1}(x_{n-1}) = y_{n-1}$. To advance the solution from x_{n-1} to x_n, we obtain a new degree m approximating polynomial $P_n(x)$ from the previous polynomial $P_{n-1}(x)$ by the relation

$$P_n(x) = P_{n-1}(x) + \delta_n C((x - x_n)/h),$$

where C is a fixed polynomial of degree m characteristic of the particular m-step method employed and δ_n is chosen on each step to satisfy $P_n'(x_n) = f(x_n, P_n(x_n))$.

The above formalism differs slightly from that of Wallace and Gupta (1973) in that the present formalism defines the polynomial C to be independent of h. It was shown in Wallace and Gupta (1973) that the method of solution described above is exactly equivalent to the classical m-step method. Any method which can be described in the formalism of Henrici (1962), which is consistent and of order m, can be described in our formalism by suitable choice of C.

In modifying $P_{n-1}(x)$ by the addition of some multiple of $C((x - x_n)/h)$ to produce $P_n(x)$, we would normally hope to produce a $P_n(x)$ which retained as much information as possible about the behavior of the function y for $x \leqslant x_{n-1}$. We, therefore, expect that the correction $\delta_n C((x - x_n)/h)$ will in some sense be close to zero for $x \leqslant x_{n-1}$, at least in the range $x_{n-m} \leqslant x \leqslant x_{n-1}$. Equivalently, we expect the polynomial $C(x)$ to be in some sense small for $x \leqslant -1$, at least in the range $-m \leqslant x \leqslant -1$. For instance, in our formalism, the Adams-Moulton formula of order m has

$$C(-1) = 0, \quad C'(-k) = 0, \quad k = 1, 2, \ldots, m-1;$$

and the stiff formula of Gear (1969) has

$$C(-k) = 0, \quad k = 1, 2, \ldots, m.$$

Our search for new formulae has been directed towards other ways of choosing C to approximate zero for values of $x \leqslant -1$. In Wallace and Gupta (1973), we chose C to have small values in this range in an exponentially-weighted least squares sense and also in an absolute magnitude sense. We now present further methods choosing C to be small in absolute magnitude and also methods which choose C to make C' approximate zero in one or the other sense.

3. New Formulae. We present five sets of formulae, two of them based on exponentially-weighted least squares approximation and the other three based on Chebyshev approximation. Our aims in investigating new formulae are that we seek formulae with stability as close to A-stability as possible, with small truncation error coefficients and as high an order as possible.

3.1. *Exponentially-Weighted Least Squares Formulae.* The two sets of formulae we present are such that their corresponding modifier polynomials $C(x)$ have a zero at $x = -1$ and $C'(x)$ minimizes

$$\{C'(0) - 1\}^2 + \sum_{k=1}^{\infty} \nu^k \{C'(-k)\}^2$$

where the weight-factor ν is fixed $(0 < \nu < 1)$. Using formulae based on such modifier polynomials, the polynomial approximation to the solution of the differential equation will minimize (as n approaches infinity)

$$\sum_{k=0}^{\infty} \nu^k \{P_n'(x_{n-k}) - f_{n-k}\}^2.$$

Two sets of formulae are presented in Tables 4 and 5 corresponding to $\nu = 0.5$ and $\nu = 0.6$. We label them FMPD50 and FMPD60 because these polynomials (or rather their derivates) are called 'Fading Memory Polynomials' by Morrison (1969), who also discusses how to derive them. The details of the stability and truncation error of these formulae are presented in Table 1.

3.2. *Chebyshev Approximation Formulae.* In Wallace and Gupta (1973), we presented a set of formulae based on a Chebyshev approximation to $y = 0$ on the range $(-B, 0)$, where B is some suitably chosen positive real x-value. These formulae are almost A-stable up to order 6 (label them CHEB1) but the truncation error coefficients of these formulae are quite large. It was therefore thought to be worthwhile to investigate Chebyshev polynomials approximating $y = 0$ on ranges $(-B, -1)$ and $(-B, -0.5)$.

Three sets of formulae are presented. The first set provides a Chebyshev approximation to $y = 0$ on the range $(-B, -1)$. These formulae do not have very good stability and are included only because their truncation errors are quite small. We label these formulae as CHEB2. The next set provides an approximation on the range $(-B, -0.5)$ and is labelled CHEB3. The third set is such that the corresponding modifier polynomial has a zero at $x = -1$ and its derivative provides a Chebyshev approximation on the range $(-B, -0.5)$. We label this last set as CHEB4. Various other formulae have been studied, and the ones which we are presenting here were thought to be more useful.

m order	FMPD50			FMPD60		
	K_{m+1}	α	D	K_{m+1}	α	D
1	0.695	A-stable		0.50	A-stable	
2	1.05	A-stable		1.56	A-stable	
3	1.73	89.0	-0.007	3.79	89.5	-0.004
4	2.70	86.0	-0.052	8.15	87.0	-0.026
5	3.93	82.5	-0.156	16.62	84.2	-0.074
6	5.61	78.3	-0.383	33.00	81.3	-0.156
7		unstable		64.70	78.5	-0.284
8		unstable		126.58	75.2	-0.510
9		unstable		248.77	71.4	-1.240

TABLE 1

Truncation error coefficients and stability parameters for formulae FMPD50 and FMPD60

Order	CHEB1				CHEB3			
	B	K_{m+1}	α	D	B	K_{m+1}	α	D
3	9.0	0.375	89.5	-0.006	4.0	0.15	86.7	-0.112
4	15.75	1.83	89.0	-0.012	6.9	0.37	84.4	-0.152
5	24.6	13.75	88.8	-0.013	10.5	1.09	82.7	-0.183
6	35.6	136.79	88.6	-0.013	15.0	4.23	81.6	-0.189
7	Not studied		-	-	22.5	44.31	80.8	-0.144

TABLE 2

Details of Chebyshev approximation formulae CHEB1 and CHEB3

The details of the truncation error and stability of formulae CHEB1, CHEB2, CHEB3 and CHEB4 are presented in Tables 2 and 3. The details of CHEB1 are included to emphasize that $A(\alpha)$-stable formulae for almost all values of $\alpha \in [0, \pi/2)$ do exist for orders up to 6. The coefficients of these formulae are not presented since these are easy to obtain. (Formulae of order 2 are not included because these turned out to be the trapezoidal rule.)

3.3. For the sake of comparison, in Appendix A we include the details of the truncation error and stability of the stiff formulae used by Gear.

Order	CHEB2				CHEB4			
	B	K_{m+1}	α	D	B	K_{m+1}	α	D
3	1.9	0.08	77.6	-1.49	4.5	0.187	87.0	-0.095
4	2.9	0.07	56.0	-6.19	9.0	0.558	85.0	-0.291
5	4.5	0.114	39.0	-5.11	15.5	2.858	84.6	-0.326
6	7.5	0.497	30.5	-3.35	24.5	23.466	85.0	-0.185

TABLE 3

Details of Chebyshev approximation formulae CHEB2 and CHEB4

$m=1$	2	3	4	5	6
c_0	-0.8333333E0	-0.7023810E0	-0.6027778E0	-0.5287186E0	-0.4742835E0
c_2	-0.1666667E0	-0.3214286E0	-0.4611111E0	-0.5846774E0	-0.6927249E0
c_3		-0.2380952E-1	-0.6666667E-1	-0.1232079E0	-0.1884921E0
c_4			-0.2777778E-2	-0.1008065E-1	-0.2265212E-1
c_5				-0.2688172E-3	-0.1190476E-2
c_6					-0.2204586E-4

TABLE 4

Coefficients of formulae FMPD50

Modifier polynomial $C(x) = \Sigma_{i=0}^{m} c_i x^i$, $c_1 = -1.0$

Also, at the suggestion of the referee, we present in Appendix B the coefficients of the conventional representation of the formulae CHEB1, CHEB2, CHEB3, CHEB4, FMPD50 and FMPD60.

4. Testing.

4.1. Recently Enright, Hull and Lindberg (1975) have tested five methods for solving stiff differential equations. The methods tested include a slightly modified version of the subroutine DIFSUB of Gear, two methods based on Runge-Kutta formulae, a variable-order method based on the second derivative multistep formulae developed by Enright (1974) and a fourth-order method based on the trapezoidal rule with extrapolation developed by Lindberg (1971). The main conclusion of this study is that generally the methods based on Runge-Kutta formulae are unreliable (except for solving linear problems). Also the modified subroutine DIFSUB has been found to be efficient on all problems except when some of the eigenvalues of the Jacobian are close to the imaginary axis. This leads us to believe that if the stiff multistep formulae used in DIFSUB were replaced by some other multistep formulae of higher order and better stability, the resulting subroutine may be significantly better than the other available methods.

m=	2	3	4	5
c_0	-0.8750000E0	-0.7687075E0	-0.6801471E0	-0.6076182E0
c_2	-0.1250000E0	-0.2448980E0	-0.3578431E0	-0.4626417E0
c_3		-0.1360544E-1	-0.3921569E-1	-0.7479374E-1
c_4			-0.1225490E-2	-0.4626417E-2
c_5				-0.9252834E-4

m=	6	7	8	9
c_0	-0.5490005E0	-0.5020428E0	-0.4645855E0	-0.4346992E0
c_2	-0.5587451E0	-0.6461482E0	-0.7252434E0	-0.7966720E0
c_3	-0.1181525E0	-0.1671921E0	-0.2200572E0	-0.2752128E0
c_4	-0.1083065E-1	-0.2015679E-1	-0.3266631E-1	-0.4823232E-1
c_5	-0.4296455E-3	-0.1188104E-2	-0.2540317E-3	-0.4634746E-2
c_6	-0.5967299E-5	-0.3277528E-4	-0.1043036E-3	-0.2515721E-3
c_7		-0.3344416E-6	-0.2116049E-5	-0.7605484E-5
c_8			-0.1653164E-7	-0.1182200E-6
c_9				-0.7297528E-9

TABLE 5

Coefficients of formulae FMPD60

Modifier polynomial $C(x)$ of degree $m = \Sigma_{i=0}^{m} c_i x^i$, $c_1 = -1.0$

Our aim in testing was to compare the several new multistep formulae we have developed with the stiff formulae used by Gear in DIFSUB (1971). Our testing is not very extensive; in fact, we have tested the formulae on only one test problem while Enright et al. (1975) have used several test problems. We can, therefore, expect only limited information from the testing.

The formulae tested are discussed in Section 4.2 and the algorithm used is discussed in 4.3. In Section 4.4, we present the test problem and the test results.

4.2. *Formulae.* The following sets of multistep formulae were tested. For each set we give the maximum order and the stability parameter α. A value of α for a set is the maximum value of α such that all the formulae in that set are stable within the wedge $\pm\, \alpha$ in the $h\lambda$-plane. Details of the individual formulae are given in the corresponding references.

(a) FLS–formulae based on finite least squares as presented in Gupta and Wallace (1975). Maximum order = 8. Stability parameter $\alpha = 63.5$ deg.

(b) BDF–stiff formulae used by Gear in DIFSUB (1971). Maximum order = 6. Stability parameter $\alpha = 17$ deg.

Formulae		EPS = 10^{-3}	EPS = 10^{-5}	EPS = 10^{-7}
(a) FLS	NS/NF/NJ	87/203/16	170/407/19	288/599/25
	HE/OE	0.40/7	0.227/8	0/129/7
(b) BDF	NS/NF/NJ	95/206/14	191/497/17	309/684/24
	HE/OE	0.425/6	0.213/6	0.106/6
(c) FMP25	NS/NF/NJ	152/340/21	218/455/20	317/765/24
	HE/OE	0.453/8	0.251/8	0.142/8
(d) FMPD50	NS/NF/NJ	221/500/22	328/765/18	528/1207/17
	HE/OE	0.295/6	0.134/6	0.0669/6
(e) FMPD60	NS/NF/NJ	363/910/29	449/1139/27	592/1407/26
	HE/OE	0.368/9	0.195/9	0.113/9
(f) CHEB1	NS/NF/NJ	113/251/9	347/737/17	618/1298/24
	HE/OE	0.237/4	0.08/4	0.049/6
(g) CHEB2	NS/NF/NJ	89/197/14	182/408/19	354/956/21
	HE/OE	0.394/5	0.181/5	0.0882/6
(h) CHEB3	NS/NF/NJ	103/268/14	225/480/21	415/922/25
	HE/OE	0.283/5	0.151/6	0.075/7
(i) CHEB4	NS/NF/NJ	133/284/14	246/522/22	513/1087/24
	HE/OE	0.223/3	0.126/6	0.0576/6

TABLE 6

(Eigenvalues $- 500 \pm 0i$)

(c) FMP25—fading memory formulae with the weight-factor $\nu = 0.25$ as presented in Wallace and Gupta (1973). Maximum order = 8. Stability parameter $\alpha = 16$ deg.

(d) FMPD50, FMPD60, CHEB1, CHEB2, CHEB3 and CHEB4 presented in this paper.

4.3. *Algorithm.* The algorithm being used is a modified version of DIFSUB of Gear. The following changes were incorporated. We assume that the reader is familiar with DIFSUB of Gear (1971).

(a) PR1, PR2, and PR3 are the factors by which the step-size is changed if order $p - 1$, the present order p or order $p + 1$ is used, respectively. These are computed as follows

$$\mathrm{PR2} = 1.05\,(10\,\mathrm{D}/\mathrm{E})^{\frac{1}{2}(p+1)},$$

$$\mathrm{PR1} = 1.05\,(10\,\hat{\mathrm{D}}/\mathrm{EDWN})^{\frac{1}{2}p},$$

$$\mathrm{PR3} = 1.05\,(10\,\tilde{\mathrm{D}}/\mathrm{EUP})^{\frac{1}{2}(p+2)}.$$

Formulae		EPS = 10^{-3}	EPS = 10^{-5}	EPS = 10^{-7}
(a) FLS	NS/NF/NJ	91/210/15	178/423/18	316/676/25
	HE/OE	0.402/7	0.227/8	0.139/8
(b) BDF	NS/NF/NJ	92/189/13	183/479/16	363/824/18
	HE/OE	0.442/6	0.215/6	0.107/6
(c) FMP25	NS/NF/NJ	137/369/21	218/524/21	352/864/25
	HE/OE	0.453/8	0.243/8	0.141/8
(d) FMPD50	NS/NF/NJ	177/396/14	297/674/14	531/1487/12
	HE/OE	0.291/6	0.135/6	0.0649/6
(e) FMPD60	NS/NF/NJ	270/672/19	372/881/20	510/1325/17
	HE/OE	0.373/9	0.196/9	0.110/9
(f) CHEB1	NS/NF/NJ	148/310/11	304/666/16	724/1562/31
	HE/OE	0.187/3	0.100/5	0.047/6
(g) CHEB2	NS/NF/NJ	87/187/13	184/408/13	375/1000/18
	HE/OE	0.397/5	0.175/5	0.0883/6
(h) CHEB3	NS/NF/NJ	129/265/14	228/486/23	445/1128/21
	HE/OE	0.259/4	0.151/6	0.076/7
(i) CHEB4	NS/NF/NJ	128/269/14	287/584/17	548/1157/22
	HE/OE	0.241/4	0.103/4	0.0584/6

TABLE 7

(Eigenvalues − $50 \pm 50i$)

D, $\hat{\mathrm{D}}$, $\tilde{\mathrm{D}}$ are the squares of the error estimates at order p, $p-1$ and $p+1$, respectively, and E, EDWN, EUP are the squares of the error requirements (times some constants) at orders $p, p-1$ and $p+1$, respectively.

(b) In DIFSUB if the step increase is less than 10%, then the step is not changed. We allow step change if the change is more than 2.5%.

(c) Necessary changes to allow higher-order formulae.

These changes may seem arbitrary. The aim was to change the algorithm so that it will tend to go to as high an order as possible.

4.4. *Test Problem and Results.* The test problem was

$$y_1' = vy_1 - uy_2 + (-v + u + 1)e^x, \qquad y_2' = uy_1 - vy_2 + (-v - u + 1)e^x,$$

$$y_1(0) = 2, \qquad y_2(0) = 1.$$

Formulae		EPS = 10^{-3}	EPS = 10^{-5}	EPS = 10^{-7}
(a) FLS	NS/NF/NJ	140/340/21	294/660/34	789/1953/34
	HE/OE	0.375/6	0.227/8	0.043/4
(b) BDF	NS/NF/NJ	147/342/17	660/1580/34	1202/2943/26
	HE/OE	0.455/6	0.213/6	0.031/4
(c) FMP25	NS/NF/NJ	507/1223/31	322/749/28	646/1576/32
	HE/OE	0.431/8	0.243/8	0.136/8
(d) FMPD50	NS/NF/NJ	224/570/18	418/1038/16	796/2122/18
	HE/OE	0.292/6	0.132/6	0.0698/6
(e) FMPD60	NS/NF/NJ	346/771/27	453/1024/28	740/1961/21
	HE/OE	0.357/9	0.194/9	0.113/9
(f) CHEB1	NS/NF/NJ	204/479/14	515/1203/23	1127/2492/31
	HE/OE	0.177/3	0.085/4	0.0446/6
(g) CHEB2	NS/NF/NJ	134/315/18	454/1192/58	1018/2553/49
	HE/OE	0.376/5	0.063/3	0.0273/4
(h) CHEB3	NS/NF/NJ	159/403/23	357/834/24	712/1628/24
	HE/OE	0.282/5	0.148/5	0.081/6
(i) CHEB4	NS/NF/NJ	172/382/19	417/1058/25	844/2068/29
	HE/OE	0.240/4	0.110/5	0.066/6

TABLE 8

(Eigenvalues $-10 \pm 50i$)

We want the solution on the interval. The exact solution is (0, 20).

$$y_1 = c_1 e^{vx} \cos(ux + c_2) + e^x, \qquad y_2 = c_1 e^{vx} \sin(ux + c_2) + e^x.$$

For the given initial conditions $c_1 = 1, c_2 = 0$.

The eigenvalues of the Jacobian of the system of equations are $v \pm iu$. We choose four sets of values for v and u

(1) $v = -500, u = 0,$
(2) $v = -50, u = 50,$
(3) $v = -10, u = 50,$
(4) $v = -10, u = 100.$

The formulae were tested for accuracy requirements (EPS) of 10^{-3}, 10^{-5}, 10^{-7}.

The results of the numerical testing are presented in Tables 6 to 9. We have tabulated the number of steps (NS), the number of function evaluations (NF), the number of Jacobian evaluations (NJ), the step-size at exit (HE) and the order of the

Formulae		EPS = 10^{-3}	EPS = 10^{-5}	EPS = 10^{-7}
(a) FLS	NS/NF/NJ	208/498/33	474/1142/38	1568/3597/26
	HE/OE	0.40/7	0.226/8	0.0195/3
(b) BDF	NS/NF/NJ	2473/5849/134	390/1001/20	2811/6734/131
	HE/OE	0.0085/5	0.222/6	0.0085/6
(c) FMP25	NS/NF/NJ	2707/6639/32	2814/6531/36	2124/5143/47
	HE/OE	0.0071/4	0.0078/6	0.144/8
(d) FMPD50	NS/NF/NJ	276/708/19	629/1604/23	1216/2989/21
	HE/OE	0.296/6	0.148/6	0.0711/6
(e) FMPD60	NS/NF/NJ	3313/9666/25	3340/7382/86	1219/3238/37
	HE/OE	0.0061/6	0.0073/7	0.111/9
(f) CHEB1	NS/NF/NJ	279/661/23	770/1720/35	1707/3939/39
	HE/OE	0.193/4	0.091/6	0.0515/6
(g) CHEB2	NS/NF/NJ	1838/4456/248	709/1815/52	2301/5556/92
	HE/OE	0.010/4	0.115/4	0.0125/4
(h) CHEB3	NS/NF/NJ	235/593/27	549/1298/36	1150/2666/34
	HE/OE	0.281/5	0.148/6	0.081/6
(i) CHEB4	NS/NF/NJ	256/669/22	623/1354/34	1413/3218/37
	HE/OE	0.211/3	0.109/5	0.056/6

TABLE 9

(Eigenvalues $-10 \pm 100i$)

method being used at exit (OE). The last two parameters, HE and OE, are generally not compared, but in our opinion they provide very useful information. Comparing HE, we can get some idea of how various formulae would have performed had the integration interval been larger. Comparing OE, we can see how the variable order algorithm is working for the various formulae.

We do not include details about the errors in the numerical solution for all test cases. In Table 10 we do, however, give the ratio of the maximum relative error in the numerical solution to the required error (EPS) for eigenvalues $-50 \pm 50i$.

5. **Concluding Remarks.** (1) FLS seems to be one of the better formulae. In most cases it is better than the rest of the formulae, and for eigenvalues $-10 \pm 50i$ and $-10 \pm 100i$ the degradation in its performance is not too bad.

(2) The algorithm seems to have suited some formulae more than others, and it would be expected that the performance of at least some formulae could be substantially improved by 'tuning' the algorithm to the formulae. Also, the algorithm

Formulae	EPS = 10^{-3}	EPS = 10^{-5}	EPS = 10^{-7}
FLS	0.54	1.01	1.78
BDF	0.55	3.05	2.12
FMP25	1.09	1.51	1.39
FMPD50	1.50	1.67	3.53
FMPD60	2.46	2.34	3.56
CHEB1	2.10	6.82	6.02
CHEB2	8.73	9.80	6.17
CHEB3	2.20	3.60	7.40
CHEB4	1.25	5.70	8.50

TABLE 10

Ratio of the maximum relative error to EPS for eigenvalues $-50 \pm 50i$

definitely needs modification if it is to be used with high-order formulae (order $\geqslant 8$). This is very well demonstrated by the performance of FMPD60 at EPS = 10^{-3} and 10^{-5} ($\lambda = -10 \pm 100i$) and of FMP25 at EPS = 10^{-3} ($\lambda = -10 \pm 50i$), among others. The poor performance of these two formulae at the cases referred to was due to corruption of the derivatives of the approximating polynomial when the step-size had to be reduced. Also when higher-order formulae are being used, the step-change takes place less frequently since at least $m + 1$ steps (for order m) must be taken between two step-size changes.

(3) Krogh (1973) has remarked that the importance of A-stability in practical computation is doubtful. To find whether requirements similar to A-stability are useful, we thought of comparing CHEB1 and FLS. CHEB1 are almost A-stable while FLS have the stability parameter $\alpha = 63.5$ for the 8th-order formula. Both the formulae were tested for eigenvalues $-10 \pm 0i$, $-10 \pm 25i$, $-10 \pm 50i$ and $-10 \pm 100i$ (for EPS = 10^{-7}). The numbers of steps required by FLS were 241, 367, 789 and 1568, respectively. CHEB1 needed 563, 783, 1127 and 1707 steps for these eigenvalues, respectively. The ratio of the number of steps at $-10 \pm 100i$ to the number of steps at $-10 \pm 0i$ comes out to be 6.5 for FLS and 3.03 for CHEB1. The ratio comes out to be more than 10 for stiff formulae used by Gear. This shows the usefulness of A-stability or a similar requirement.

(4) Many of the new formulae presented in this paper have performed much better than the stiff methods used in DIFSUB when the eigenvalues of the Jacobian are close to the imaginary axis. Further investigation is required, and suitable algorithm(s) are being designed for these new formulae.

6. Acknowledgments. The author is grateful to the referee and Professor C. S. Wallace for several useful suggestions.

Appendix A

Order	K_{m+1}	α	D
2	0.333	A-stable	
3	0.250	86.0	-0.1
4	0.200	73.5	-0.7
5	0.167	51.8	-2.4
6	0.143	17.2	-6.1

TABLE A1

Details of the truncation error and stability of the stiff formulae used by Gear

Appendix B

A k-step multistep formula is usually represented by

$$\alpha_k y_{n+k} + \alpha_{k-1} y_{n+k-1} + \cdots + \alpha_0 y_n = h\{\beta_k f_{n+k} + \beta_{k-1} f_{n+k-1} + \cdots + \beta_0 f_n\}.$$

The coefficients α_i and β_i are now presented for various formulae studied in this paper.

$m=$	3	4	5	6
α_0	-0.473245	0.457734	-0.4538100	0.454151
α_1	1.814802	-2.204274	2.632823	-3.454151
α_2	-2.341557	4.010774	-6.138831	8.746665
α_3	1.0	-3.264234	7.191439	-13.280660
α_4		1.0	-4.231530	11.380330
α_5			1.0	-5.217959
α_6				1.0
β_0	0.225649	-0.221578	0.218120	-0.215042
β_1	-0.412208	0.628302	-0.832033	1.028761
β_2	-0.181752	-0.256324	0.859755	-1.636942
β_3	0.500000	-0.618016	0.361547	0.433327
β_4		0.492188	-1.096034	1.493303
β_5			0.492000	-1.597493
β_6				0.494444

TABLE B1

Coefficients of the formulae CHEB1

$m=$	3	4	5	6
α_0	-0.074018	0.065599	-0.072531	0.102289
α_1	0.173317	-0.324563	0.444825	-0.739465
α_2	-1.099299	0.534187	-1.156848	2.325060
α_3	1.0	-1.275223	1.675396	-4.155048
α_4		1.0	-1.890842	4.600784
α_5			1.0	-3.133620
α_6				1.0
β_0	-0.003701	0.003895	-0.005078	0.009234
β_1	0.028262	-0.015666	0.026406	-0.063495
β_2	0.490674	0.032236	-0.048456	0.192518
β_3	0.459483	0.471925	0.016838	-0.353706
β_4		0.425753	0.179947	0.478237
β_5			0.424294	-0.538770
β_6				0.456529

TABLE B2

Coefficients of the formulae CHEB2

$m=$	3	4	5	6	7
α_0	-0.185455	0.184774	-0.179454	0.179042	-0.216535
α_1	0.905455	-1.043426	1.181554	-1.350347	1.811553
α_2	-1.720000	2.343309	-3.219835	4.338731	-6.578664
α_3	1.0	-2.484657	4.550800	-7.612603	13.450670
α_4		1.0	-3.333064	7.699203	-16.729830
α_5			1.0	-4.254026	12.661780
α_6				1.0	-5.398978
α_7					1.0
β_0	0.071212	-0.066214	0.063818	-0.062260	0.061884
β_1	-0.241515	0.266937	-0.315183	0.367262	-0.394217
β_2	0.153030	-0.275804	0.500436	-0.775838	0.913882
β_3	0.482727	-0.211413	-0.058440	0.507655	-0.647321
β_4		0.475714	-0.597852	0.539746	-0.950950
β_5			0.469246	-1.027645	2.265066
β_6				0.467427	-1.740045
β_7					0.493668

TABLE B3

Coefficients of the formulae CHEB3

$m=$	3	4	5	6
α_0	-0.058824	0.045152	-0.045157	0.054841
α_1	0.647059	-0.610052	0.645018	-0.750922
α_2	-1.588235	1.194454	-2.489128	3.276303
α_3	1.0	-2.379641	4.196909	-6.835382
α_4		1.0	-3.307642	7.567873
α_5			1.0	-4.312712
α_6				1.0
β_1	-0.215686	0.207516	-0.201392	0.191665
β_2	0.196079	-0.397428	0.580106	-0.721944
β_3	0.490196	-0.142936	-0.247618	0.701000
β_4		0.472955	-0.574118	0.437835
β_5			0.469943	-1.080419
β_6				0.475331

TABLE B4
Coefficients of the formulae CHEB4 ($\beta_0 = 0$)

$m=$	2	3	4	5	6
α_0	0.666667	-0.428571	0.266667	-0.161290	0.095238
α_1	-1.666667	1.714286	-1.466667	1.129033	-0.809524
α_2	1.0	-2.285714	3.066667	-3.225807	2.936508
α_3		1.0	-2.866667	4.677419	-5.793650
α_4			1.0	-3.419355	6.523809
α_5				1.0	-3.952381
α_6					1.0
β_1	-0.500000	0.202381	-0.041667	-0.034454	0.062996
β_2	0.833333	-0.761905	0.386111	-0.008691	-0.259843
β_3		0.702381	-0.880556	0.472043	0.219599
β_4			0.602778	-0.925358	0.459458
β_5				0.528719	-0.940619
β_6					0.474284

TABLE B5
Coefficients of the formulae FMPD50 ($\beta_0 = 0$)

$m=$	2	3	4	5
α_0	0.750000	-0.551020	0.397059	-0.281055
α_1	-1.750000	2.020408	-1.985294	1.780014
α_2	1.0	-2.469388	3.750000	-4.559334
α_3		1.0	-3.161765	5.891742
α_4			1.0	-3.831367
α_5				1.0
β_1	-0.625000	0.360544	-0.182598	0.060103
β_2	0.875000	-1.047619	0.854167	-0.518838
β_3		0.768708	-1.322304	1.349156
β_4			0.680147	-1.495937
β_5				0.607618

TABLE B6

Coefficients of the formulae FMPD60 up to order 5 ($\beta_0 = 0$)

$m=$	6	7	8	9
α_0	0.195757	-0.134399	0.079679	-0.061082
α_1	-1.500805	1.209591	-1.021489	0.712630
α_2	4.857679	-4.733834	4.631305	-3.755304
α_3	-8.482814	10.428370	-11.720660	11.718750
α_4	8.412728	-13.942660	19.159950	-23.828010
α_5	-4.482546	11.292290	-20.811210	32.686600
α_6	1.0	-5.119361	14.439180	-30.199020
α_7		1.0	-5.756765	18.088800
α_8			1.0	-6.363351
α_9				1.0
β_1	-0.001316	-0.035643	0.105441	-0.058066
β_2	0.174028	0.114800	-0.346343	0.461995
β_3	-0.897058	0.152331	0.471950	-1.481000
β_4	1.785482	-1.202215	-0.030235	2.327339
β_5	-1.605839	2.149950	-1.332364	-1.312298
β_6	0.549001	-1.679581	2.402619	-1.309989
β_7		0.502043	-1.738357	2.724582
β_8			0.464585	-1.787282
β_9				4.346992

TABLE B7

Coefficients of the formulae FMPD60 of order greater than 5 ($\beta_0 = 0$)

Department of Computer Science
Monash University
Clayton, Victoria 3168, Australia

1. W. H. ENRIGHT, T. E. HULL & B. LINDBERG, "Comparing numerical methods for stiff systems of O.D.E.'s," *BIT*, v. 15, 1975, pp. 10–48.

2. W. H. ENRIGHT, "Second derivative multistep methods for stiff ordinary differential equations," *SIAM J. Numer. Anal.*, v. 11, 1974, pp. 321–331. MR 50 #3574.

3. C. W. GEAR, "The automatic integration of stiff ordinary differential equations (with discussion)," *Information Processing* 68 (Proc. IFIP Congress, Edinburgh, 1968), Vol. I: *Mathematics, Software,* North-Holland, Amsterdam, 1969, pp. 187–193. MR 41 #4808.

4. C. W. GEAR, "Algorithm 407–DIFSUB for solution of ordinary differential equations," *Comm. ACM,* v. 14, 1971, pp. 185–190.

5. G. K. GUPTA & C. S. WALLACE, "Some new multistep methods for solving ordinary differential equations," *Math. Comp.*, v. 29, 1975, pp. 489–500.

6. P. HENRICI, "Discrete variable methods in ordinary differential equations," Wiley, New York, 1962. MR 24 #B1772.

7. T. E. HULL, W. H. ENRIGHT, B. M. FELLEN & A. E. SEDGWICK, "Comparing numerical methods for ordinary differential equations," *SIAM J. Numer. Anal.*, v. 9, 1972, pp. 603–6 → errata, *ibid.*, v. 11, 1974, p. 681. MR 50 #3577.

8. F. T. KROGH, "On testing a subroutine for the numerical integration of ordinary differential equations," *J. ACM,* v. 20, 1973, pp. 545–562.

→ B. LINDBERG, "On smoothing and extrapolation for the trapezoidal rule," *BIT*, v. 11, 1971, pp. 29–52. MR 43 #7074.

10. N. MORRISON, *Introduction to Sequential Smoothing and Prediction*, McGraw-Hill, New York, 1969.

11. C. S. WALLACE & G. K. GUPTA, "General linear multistep methods to solve ordinary differential equations," *Austral. Comput. J.*, v. 5, 1973, pp. 62–69.

12, O. B. WIDLUND, "A note on unconditionally stable linear multistep methods," *BIT*, v. 7, 1967, pp. 65–70. MR 35 #6373.