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Some New Multistep Methods for Solving Ordinary Differential Equations

By G. K. Gupta and C. S. Wallace

Abstract. Three sets of linear multistep formulae for solving stiff and nonstiff ordinary differential equations are presented. Two of the sets are based on Adams-Moulton and stiff formulae used by Gear [1969]. A third set of formulae based on least-squares approximation is shown to be stiffly-stable up to order 8 and is suitable for solving stiff differential equations.

1. Introduction. The general linear multistep (m-step) method for the numerical solution of the differential equation

$$y' = f(x, y) \qquad (y \text{ a vector})$$

is conventionally described by the equation

$$\begin{aligned} &\alpha_m y_{n+m} + \alpha_{m-1} y_{n+m-1} + \cdots + \alpha_0 y_n \\ &\qquad = h(\beta_m f_{n+m} + \beta_{m-1} y_{n+m-1} + \cdots + \beta_0 f_n), \end{aligned} \tag{1.1}$$

where h is the step size in x, assumed constant, y_k is the computed value of y at $x_k = kh$, and $f_k = f(x_k, y_k)$.

The method described by (1.1) is explicit if $\beta_m = 0$, and implicit otherwise. As usually applied, Eq. (1.1) is solved to give y_{n+m} as a function of preceding y and f values.

An analysis of such methods is given by Henrici [1962], who concentrates on two special cases of the general method. The first, which he describes as methods based on integration, have only one nonzero α (in addition to α_m). The second described as methods based on differentiation, have only one nonzero β (β_m if the method is implicit). The latter case has recently received attention arising from the work of Gear [1969] who has shown that methods of this kind may be useful for stiff systems, whereas the former includes, *inter alia,* the Adams methods.

Investigation of methods not falling into either of these classes has been, perhaps, inhibited by the fact that, while the general m-step method is described by $2m + 1$ parameters, it is known (Dahlquist [1956]) that an m-step method can have satisfactory

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stability only if its order does not exceed $m + 1$ (m odd) or $m + 2$ (m even). A method is said to be of order q if it is exact for equations whose true solution is a polynomial of degree q or less. The requirement that an m-step method be of order m yields $(m + 1)$ conditions on its α and β parameters, leaving the method with m degrees of freedom. Complete exploration of the methods encompassed by these degrees of freedom is difficult in the formalism of Eq. (1.1) which leads to rather complicated expressions for the α and β parameters in terms of degrees of freedom. It was shown by Wallace and Gupta [1973] that these m-degrees of freedom can be conveniently isolated by representing the method by a polynomial $C(x)$ of degree m, which we have called a 'modifier polynomial'. The relation between the coefficients of $C(x)$ and the coefficients α and β of (1.1) has been shown by Wallace and Gupta [1973]. Each multistep method can be represented by a polynomial $C(x)$ and, for the methods used by Gear [1969], we have

$$C(x) = (x + 1)(x + 2) \cdots (x + m)/m! . \tag{1.2}$$

For Adams-Moulton methods, $C(x)$ is such that

$$C(x) = 0 \quad \text{at } x = -1$$

and

$$C'(x) = (x + 1)(x + 2) \cdots (x + m - 1); \qquad m \geqslant 2.$$

Hence, for $m = 2$, $C(x) = (x + 1)^2$.

Representation of multistep methods by modifier polynomials leads to computer algorithms similar to that of Nordsieck [1962] and Gear [1971a].

The main components of an algorithm to solve ODE using multistep methods are the starting method, method of solving the implicit equation, the multistep method (or formula. We use both terms to mean the same thing.), the technique used to handle variable steps and the scheme used to select step sizes. In this paper, we only consider the formula part of the whole algorithm. However, existing algorithms, such as that of Gear [1971b], are applicable to the new formulae we will present.

The formulae being investigated can be divided into two classes: for stiff equations and for nonstiff equations. The stability requirements for the two classes are different, and, for nonstiff equations, we only require that, for small $h\lambda$, the dominant root of the polynomial

$$\rho(r) - h\lambda\sigma(r) = 0, \tag{1.3}$$

where

$$\rho(r) = \sum_{i=0}^{m} \alpha_i r^i \quad \text{and} \quad \sigma(r) = \sum_{i=0}^{m} \beta_i r^i$$

be approximately equal to the solution, i.e., $e^{h\lambda}$. This is described as relative stability by Gear [1969]. In solving stiff equations, we require that the method be stiffly-stable. A method is stiffly-stable if the method is absolutely stable (i.e., gives convergent solutions) in R_1 ($\mathrm{Re}(h\lambda) \leqslant D$) and gives accurate solutions in R_2 ($D < \mathrm{Re}(h\lambda) < \alpha^*$, $|I_m(h\lambda)| < \theta$) as shown in Fig. 1.

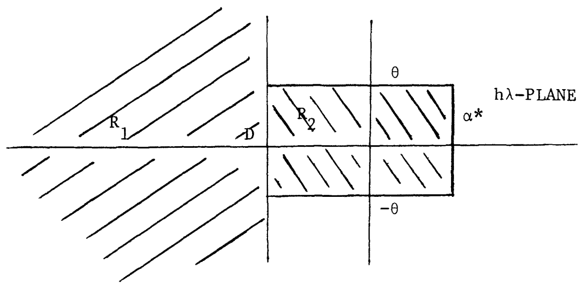

FIGURE 1

Other requirements have been suggested for solving stiff equations, e.g., A-stability suggested by Dahlquist [1963] requires that method be absolutely stable in the negative half of $h\lambda$-plane. $A(\alpha)$-stability suggested by Widlund [1967] requires that method be absolutely stable in the wedge-shaped region $S(\alpha)$ as shown in Fig. 2, for any $0 \leqslant \alpha \leqslant \pi/2$. $A(\pi/2)$-stable methods are A-stable.

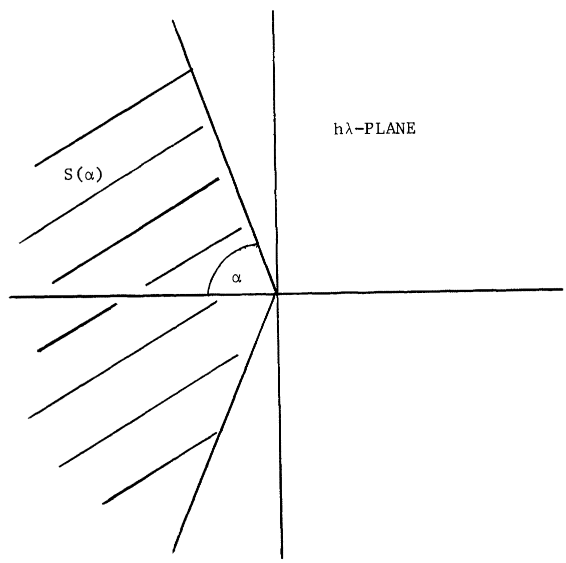

FIGURE 2

Stiff-stability implies $A(0)$-stability and hence the following results:

THEOREM 1. *For multistep methods of order greater than* 2, *no m-degree* (*m-step*) *implicit stiffly-stable method can be of order greater than m.*

THEOREM 2. *No explicit multistep method can be stiffly-stable.*

Both theorems follow from the results of Widlund [1967].

To study the stability of a method, we may plot the locus of $h\lambda = \rho(r)/\sigma(r)$ for $r = e^{i\phi}$ $(0 \leqslant \phi \leqslant 2\pi)$. We call this locus the stability curve of the method. For stiff-stability, we require that the method be absolutely stable at $h\lambda = \infty$, i.e., $\sigma(r)$ has roots within the unit circle. Based on the continuity argument, we can say that the region of $h\lambda$-plane which can be reached from $h\lambda = \infty$ without crossing the stability curve is also stable. For methods of order greater than 2, the parameter D must be a negative number and so, for stiff-stability, the stability curve must turn to the positive half of the $h\lambda$-plane. The stability curve intersects the real axis at at least $r = \pm 1$. At $r = 1$, we have $h\lambda = 0$ and so $h\lambda$ must be positive for $r = -1$. We now summarise the discussion in the following theorem:

THEOREM 3. *For an implicit linear multistep method of order greater than* 2 *to be stiffly-stable, the following conditions are necessary and sufficient*:

(i) $\rho(r)$ *has all roots within the unit circle except one simple root on the circle at* $r = 1$ (*this is root condition*),

(ii) $\alpha(r)$ *has all roots within the unit circle,*

(iii) $h\lambda$ *at* $r = -1$ *is positive,*

(iv) *the stability curve does not intersect the negative real axis.*

We assume that the stability curve does not intersect the real axis at more than the two points corresponding to $r = \pm 1$, this being the case with all the methods which have been studied so far and have satisfactory stability. For such methods, the $h\lambda$-value at $r = -1$ is a good indication of the overall stability of a particular formula. (The stability at $h\lambda = 0$ is important and so must be investigated in detail.)

Since no linear multistep method of order greater than 2 can be A-stable, we must use the criterion of stiff-stability and/or $A(\alpha)$-stability. Thus, the important parameters of the stability curve of a method used for stiff equations are D, θ (as shown in Fig. 1) and wedge angle α (as shown in Fig. 2). It is quite easy to find the wedge angle α and parameter D from a stability curve, but it is not clear from the definition of stiff-stability how θ should be obtained. In the definition of stiff-stability, we have said that in region R_2 (Fig. 1) the numerical solutions should be accurate. In our opinion, that definition needs to be made more precise by stating that in region R_2 we require that

(a) the solutions be accurate around the origin and in the subregion enclosed by the stability curve, the lines $\mathrm{Re}(h\lambda) = 0$ and $I_m(h\lambda) = \pm\,\theta$, and

(b) the solutions be absolutely stable in the subregion enclosed by the three lines $\mathrm{Re}(h\lambda) = D$, $I_m(h\lambda) = \pm\,\theta$ and the stability curve.

θ can now be obtained based on the requirement (a) of accuracy. If the stability curve is the locus of $r = e^{i\phi}$ as discussed earlier, following Gupta and Wallace [1974], we can show that

$$i\phi - h\lambda \simeq K_{m+1}(h\lambda)^{m+1} + K_{m+2}(h\lambda)^{m+2} + \cdots, \tag{1.4}$$

where $h\lambda$ is the point on the stability curve corresponding to $i\phi$ and K_{m+1}, K_{m+2} are truncation error coefficients of the formula (of order m) being used.

To find θ, we start to investigate whether relation (1.4) is being satisfied for points on the stability curve near the origin. The value of θ is then given by $I_m(h\lambda)$, where $h\lambda$ is the point closest to the origin where the relation first breaks down. We have arbitrarily taken the maximum value of θ as 0.75, assuming that we are not really interested whether θ is greater than 0.75.

For some formulae, θ will be limited by the requirement of absolute stability as explained in (b). This may happen when the stability curve touches the line $I_m(h\lambda) = \pm\theta$, as for the sixth-order method used by Gear [1969].

In this paper, rather than presenting stability curves of all the methods we study, we will present the values of D, θ and α and these, in our opinion, are sufficient to compare the stability of various methods.

In Section 2, we present new formulae for stiff and nonstiff equations based on the presently used formulae. In Section 3, we present some more new high-order formulae for stiff equations. In Section 4, the results of numerical experiments are presented and in Section 5, these results are briefly discussed.

2. **Method Based on Interpolation.** The most commonly used methods are the methods based on interpolation, that is, the Adams-Moulton methods for nonstiff differential equations and the methods used by Gear [1969] for stiff equations. We label these methods as A_m and I_m, respectively, (for degree m). Now, we will discuss how new methods may be developed from these methods.

Consider, for example, the modifier polynomial $C(x)$ of degree 3

$$C(x) = c_0 + c_1x + c_2x^2 + c_3x^3. \tag{2.1}$$

The truncation error at the nth step is $K_{m+1}h^{m+1}y^{(m+1)}(x_n)$, and K_{m+1} is given by (cf. Wallace and Gupta [1973])

$$K_{m+1} = (c_0 - c_1/2 + c_2/6)/6c_3. \tag{2.2}$$

To study the stability of the modifier polynomial of degree 3, we have from Wallace and Gupta [1973]

$$h\lambda \ (\text{at } r = -1) = \frac{c_1 - c_2}{c_0 - 0.5c_1 + 0.25c_2}. \tag{2.3}$$

Now the following observations can be made on the basis of (2.2) and (2.3):

(1) Since $\rho(r)$ is not a function of c_0, the stability of $h\lambda = 0$ is independent of c_0.

(2) If $h\lambda$ (at $r = -1$) is positive, then reducing c_0 increases the value of $h\lambda$ (at $r = -1$) till the denominator in (2.3) is equal to zero and hence $h\lambda$ (at $r = -1$) $= \infty$.

(This will happen before $c_0 = 0$ which corresponds to an explicit method.)

(3) If $h\lambda$ (at $r = -1$) is negative, then reducing c_0 reduces the (absolute) value of $h\lambda$ (at $r = -1$) till it reaches a limiting value at $c_0 = 0$.

(4) If K_{m+1} is positive, then reducing c_0 reduces K_{m+1} till $K_{m+1} = 0$.

Based on these observations we have developed some new formulae as explained below:

2.1. *For Stiff Equations.* The formulae I_m used by Gear [1969] all have $K_{m+1} > 0$ and $h\lambda$ (at $r = -1$) > 0. Thus we can improve the truncation error by reducing c_0 till the limiting case of $h\lambda$ (at $r = -1$) $= \infty$ is reached. We have done this and have thus obtained a new set of formulae which we label as I_m^*. The modifier polynomials corresponding to I_m and I_m^* have the same coefficients $c_1, c_2, \ldots, c_m$ but c_0 are different. We tabulate new values of c_0 (scaling coefficients so that $c_1 = 1$) and new values of K_{m+1}.

m=	2	3	4	5	6
c_0 for I_m	2/3	6/11	24/50	120/274	720/1764
c_0 for I_m^*	1/2	5.25/11	22.5/50	116.25/274	708.75/1764
K_{m+1} for I_m	1/3	1/4	1/5	1/6	1/7
K_{m+1} for I_m^*	1/12	1/8	11/80	13/96	57/448

TABLE 1

The stability of I_m^* was investigated and, as expected, all the stability curves satisfied the stiff-stability requirements. The stability of I_m^* is compared with that of I_m in Table 4, and we can see that, for $m = 5$ and 6, the stability of I_m^* is better than that of I_m.

2.2. *For Nonstiff Equations.* We know that the Adams-Moulton method of order 2 (A_2 or trapezoidal rule) is A-stable. For A_3, we have $h\lambda$ (at $r = -1$) $= -6$ and, for A_4, the value of $h\lambda$ (at $r = -1$) $= -3$ and so on. That is, the region of absolute stability is reducing as the order of the formula increases. Ideally, we want that the region of absolute stability be larger for higher-order formulae. While using lower-order methods, the $h\lambda$ value must be kept fairly small in order to obtain reasonable accuracy, and, hence, the large region of absolute stability of the lower-order formulae is of no use and could be reduced by reducing c_0 which in turn reduces the truncation error coefficient K_{m+1}.

We must now consider how far K_{m+1} should be reduced and how small a region of absolute stability will be sufficient. Regarding K_{m+1}, we want that the error term of $O(h^{m+2})$ should not be greater than $O(h^{m+1})$ for reasonable values of $h\lambda$. This is required because, for a general-purpose method, there is little point in eliminating errors of order m if the result is an error of order $m + 1$ which is actually larger in magnitude. The second consideration is that, for nonstiff equations, $|h\lambda|$ is not expected to exceed ½, because $|h\lambda| = ½$ will give only about 4–5 digit accuracy when a method of order 10 is used.

Based on these considerations, we have obtained new values of c_0 for the Adams-Moulton methods. We label these formulae with new value of c_0 as A_m^*. We have arbitrarily chosen $K_{m+1} = 1/96$ (for $m = 2$ to 7) for A_m^* because this value was close to satisfying the criterion we discussed above and also because having the same K_{m+1} for all m will be convenient in the algorithm.

m=	2	3	4	5	6	7
c_0 for A_m	1/2	5/12	9/24	251/720	475/1440	19087/60480
c_0 for A_m^*	41/96	37/96	517/1440	245/720	19717/60480	38049/120960
K_{m+1} for A_m	1/12	1/24	19/720	27/1440	863/60480	1375/120960
K_{m+1} for A_m^*	1/96	1/96	1/96	1/96	1/96	1/96
$h\lambda(-1)$ for A_m	∞	-6.0	-3.0	-1.8	-1.2	-0.77
$H\lambda(-1)$ for A_m^*	-6.9	-3.4	-2.2	-1.5	-1.0	-0.73

TABLE 2

We can see that as the order increases, the difference between A_m and A_m^* becomes smaller. This is because higher-order Adams-Moulton methods have quite small regions of absolute stability and also their value of K_{m+1} is small.

3. **New Methods for Stiff Equations Based on Least Squares.** As indicated in Section 2, it seems that one of the best algorithms available to solve stiff differential equations is that of Gear [1971a, b]. In Section 2, we suggested how new formulae could be obtained from the formulae used in this algorithm by Gear. Though these new formulae are more accurate and slightly more stable, there still remains room for further improvement. Our aims in investigating other formulae are twofold. First, we want that the stability curves of the new formulae approach A-stability as closely as possible, i.e., the value of D should be smaller, and α and θ should be larger than for methods used by Gear [1969]. Secondly, we want that the new set of formulae be stable for as high an order as possible. Some such formulae were presented in Wallace and Gupta [1973], but, except for one set of formulae (called $L_{¼,m}$ in that paper), the truncation error was too large for the formulae to be useful.

The modifier polynomials corresponding to the new formulae we are presenting in this section have a zero at $x = -1$, and their first derivatives provide a least-squares approximation to points (0, 1), (− 1, 0), (− 2, 0), . . . , (−n, 0), ($n \geqslant m - 1$), the value of n was so chosen that the formula was stiffly stable and the truncation error was small. Morrison [1969] explains the algorithm used in obtaining these formulae based on Legendre polynomials. The coefficients c_i of the modifier polynomials $C(x)$ for these formulae are presented in the Appendix. Also presented in the appendix are the coefficients α_i, β_i for these methods.

In Table 3, we present the values of K_{m+1} for the formulae used by Gear [1969], and these new formulae we have obtained (which are labelled as L_m). We also present the values of the stability parameters D, θ, α of L_m in Table 4. In Fig. 3, we present the stability curves of methods L_m for m = 3 to 6. The stability curves of L_7 and L_8 are very close to that of L_6 and so have not been shown. Also, we have shown parts of the stability curves of I_5 and I_6 for comparison.

m=	3	4	5	6	7	8
I_m	$\frac{1}{4}$	$\frac{1}{5}$	$\frac{1}{6}$	$\frac{1}{7}$	-	-
L_m	0.104	0.15	0.28	0.602	1.6	5.0

TABLE 3

Truncation error coefficient K_{m+1} of least-squares polynomials

m	I^*_m			I_m			L_m		
	D	θ	α	D	θ	α	D	θ	α
3	-0.23	0.75	85.5	-0.1	0.75	86.0	-0.63	0.75	82.3
4	-0.85	0.75	76.0	-0.7	0.75	73.5	-1.36	0.75	74.8
5	-2.16	0.75	58.0	-2.4	0.75	51.8	-1.39	0.75	70.1
6	-4.82	0.61	26.0	-6.1	0.50	17.2	-1.75	0.75	65.7
7		Unstable			Unstable		-1.79	0.75	64.8
8		Unstable			Unstable		-1.81	0.75	63.6

TABLE 4

Stiff-stability parameters D and θ and A(α)-stability parameter α for various formulae

4. Numerical Results. As explained in Wallace and Gupta [1973], we are using an algorithm similar to DIFSUB of Gear [1971b] to test the performance of the individual formulae. The modified algorithm uses a starting procedure with a series of variable-order methods till a polynomial approximation of desired degree is obtained. After that, the step size and the modifier polynomial being used are not changed.

The test problem was

$$y' = vy_1 - wy_2 + (-v + w + 1)e^x, \quad y_2' = wy_1 + vy_2 + (-v - w + 1)e^x,$$
$$y_1(0) = 1, \quad y_2(0) = 1.$$

The exact solution is

$$y_1 = c_1 e^{vx} \cos(wx + c_2) + e^x, \quad y_2 = c_1 e^{vx} \sin(wx + c_2) + e^x$$

for the given initial conditions $c_1 = 0$, $c_2 = 0$.

The eigenvalues of the jacobian of the system of equations are $v \pm iw$. We chose $v = -80$ and $w = 8$ for testing stiff equations and $v = 1$ and $w = 0$ for testing nonstiff equations. The step size used was 1/8 for both, and the numerical solution was computed from $x = 0.0$ to $x = 10.0$.

m	A_m	A^*_m
2	1.137E-2	1.804E-3
3	6.612E-4	1.864E-4
4	4.856E-5	2.021E-5
5	4.007E-6	2.272E-6
6	3.528E-7	2.623E-7

TABLE 5

Maximum error at $x = 10.0$ for nonstiff methods ($h\lambda = 1/8$)

Table 5 gives the maximum error (maximum of errors in the solutions y_1 and y_2) at $x = 10.0$ for nonstiff formulae A_m and A^*_m and Table 6 for stiff formulae I_m, I^*_m and L_m. All computing was done on a CDC 3200 machine (48-bit word, 36-bit mantissa).

m	I_m	I^*_m	L_m
2	6.378E-5	1.746E-5	1.747E-5
3	5.656E-6	2.932E-6	2.459E-6
4	5.339E-7	3.739E-7	3.940E-7
5	5.246E-8	4.305E-8	8.123E-8
6	5.243E-9	4.700E-9	1.863E-8
7	Unstable	Unstable	5.214E-9
8	Unstable	Unstable	1.674E-9

TABLE 6

Maximum error at $x = 10.0$ for stiff methods ($h\lambda = 10 \pm i$)

5. Discussion and Conclusions. We have presented methods which are better than methods being used presently; for nonstiff equations, methods A^*_m are more accurate than the Adams-Moulton methods, especially for order $\leqslant 6$. For stiff equations, I_m^* are more accurate than the formulae used by Gear [1969] but similar to I_m are unstable for $m \geqslant 7$. L_m are high-order methods stiffly-stable for $m \leqslant 8$ and are generally more stable than I_m. We expect these new formulae to be quite useful in improving the present algorithms such as that of Gear [1971b].

Appendix. Let the modifier polynomial for $L_m = \Sigma_{j=0}^m c_j x^j$. We tabulate c_j for formulae of degree 3 to 8 ($c_1 = 1.0$).

m=	3	4	5
c_0	.4687814703E0	.4478808250E0	.4380080363E0
c_2	.6570996979E0	.7413433044E0	.7845665359E0
c_3	.1258811682E0	.2091131486E0	.2581998306E0
c_4		.1988901927E-1	.3763231522E-1
c_5			.2007056812E-2

m=	6	7	8
c_0	.4293908371E0	.4252280277E0	.4224433336E0
c_2	.8168964245E0	.8346135193E0	.8467063986E0
c_3	.5209156055E-1	.3155972849E0	.3306145264E0
c_4	.4457494121E-2	.6196227876E-1	.6917486868E-1
c_5	.1472432240E-3	.6552469094E-2	.8252267597E-2
c_6		.3540405890E-3	.5622383395E-3
c_7		.7667697333E-5	.2036050560E-4
c_8			.3039471181E-6

We also present the coefficients α_i and β_i for formulae L_m, $m = 3$ to 8. Note that $\beta_0 = 0.0$ for all formulae.

m	3	4	5	6	7	8
α_0	-0.06344	0.06512	-0.06497	0.06145	-0.06041	0.05976
α_1	0.37160	-0.41795	0.47337	-0.50752	-0.55769	-0.60984
α_2	-1.30816	1.16325	-1.48838	1.83520	-2.28502	2.79586
α_3	1.0	-1.81042	2.57568	-3.75212	5.41112	-7.54072
α_4		1.0	-2.49570	4.61546	-8.03577	13.12039
α_5			1.0	-3.25247	7.51356	-15.11693
α_6				1.0	-4.10119	11.28474
α_7					1.0	-4.99327
α_8						1.0

m	3	4	5	6	7	8
β_1	-0.09013	0.05855	-0.04857	0.04468	-0.04230	0.04053
β_2	0.37664	-0.20790	0.20319	-0.22754	0.25473	-0.28339
β_3	0.46878	0.17882	-0.24415	0.39529	-0.57313	0.78462
β_4		0.44788	-0.10763	-0.12711	0.46659	-0.97484
β_5			0.43801	-0.40868	0.26504	0.17538
β_6				0.42939	-0.75751	0.97171
β_7					0.42523	1.12422
β_8						0.42244

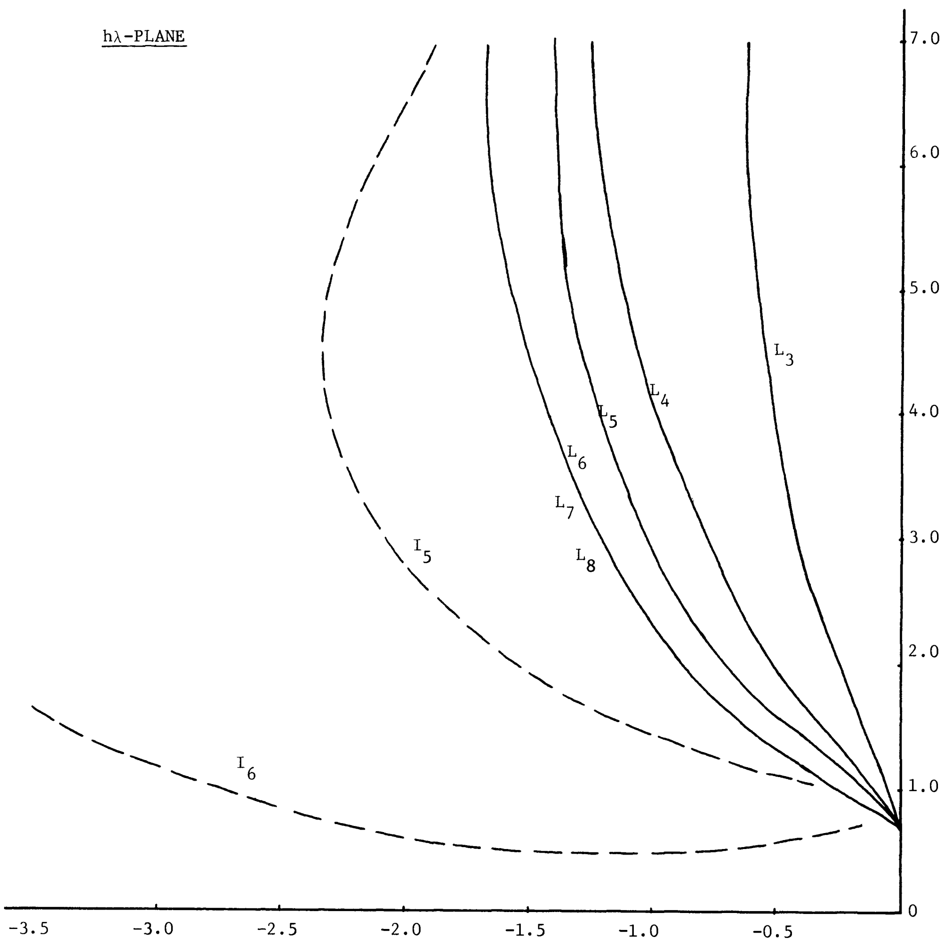

FIGURE 3. *Stability curves for some methods (stability curves for L_7 and L_8 are very close to the one for L_6)*

Department of Computer Science
Monash University
Clayton, Victoria, Australia

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