

T. E. HULL AND A. L. CREEMER[†]

The University of British Columbia, Vancouver, B.C., Canada

1. Introduction

In deciding which of the many possible predictor-corrector procedures should be used in practice, one is mainly concerned with choosing the predictor formula, the corrector formula, the step-size and the rule for iterating with the corrector formula. One would like to make these choices in such a way that the required calculation can be carried to within some prescribed accuracy, at minimum cost.

The purpose of this paper is to present a study of how the relationship between accuracy and cost depends on the choice of predictor-corrector formulas and on the iteration rule.

We assume that the differential equations being considered are fairly complicated. The cost will then be proportional to the number of evaluations per step multiplied by the total number of steps. By an evaluation we mean an evaluation of the function f(t, x) that appears in the initial-value problem being considered, namely, in

$$x' = f(t, x), \quad x(t_0) = x_0.$$
 (1)

In Section 2 some theoretical results are obtained which serve mainly to indicate that the best procedures will involve only one evaluation of f and one application of the corrector formula per step, unless extra iterations are needed to make the procedure stable.

In Section 3 experiments are described for determining whether or not extra iterations are needed. We use 1, 2, 3 and 4 iterations with each of a representative set of predictor and corrector formulas. We use each method with a range of different step-sizes and with a fairly wide variety of differential equations.

Conclusions are given in detail in Section 4. Of course, we do not expect one particular method to be best in every situation. However, it turns out that only a very few methods are consistently good. Each involves a second iteration per step, which appears to be needed for stability, and each has a high step-number, which is needed for accuracy. We recommend particularly the predictor and corrector formulas of the Adams type, with truncation errors which are proportional to h^8 or h^9 , where h is the step-size. At each step there should be two evalu-

† Present address: Shell Oil Company, Calgary, Alberta, Canada.

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ations of the function and two applications of the corrector formula. The stepsize must be chosen according to certain accuracy and stability criteria which depend on the differential equation being solved.

It should be emphasized that our conclusions are based on the assumption that f(t, x) is relatively complicated, so that the cost depends only on the total number of evaluations. We also consider only general-purpose procedures, and we therefore rule out any procedures which are applicable only in restricted circumstances.

2. Theoretical Results

We write the predictor formula as

$$y_n = \sum_{i=1}^k a_i^* y_{n-i} + h \sum_{i=1}^{k+1} b_i^* y'_{n-i}, \qquad (2)$$

and the corrector formula as

$$y_n = \sum_{i=1}^k a_i y_{n-i} + h \sum_{i=0}^k b_i y'_{n-i} .$$
(3)

The corrector formula contains the term hb_0y_n' , whereas there can, of course, be no corresponding term $hb_0^*y_n'$ in the predictor formula. Instead, we have included the extra term $hb_{k+1}^*y_{n-k-1}'$ in the predictor. This will be convenient later when we will want the predictor and corrector formulas to have truncation errors of the same degree. Meanwhile we will drop the limits from the summation signs and understand them to be as given in (2) and (3), unless otherwise specifically noted.

A predictor-corrector procedure consists in first using (2) to "predict" an approximation to $x_n = x(t_n)$, next using f(t, x) to evaluate an approximation to x_n' , and then using (3) to "correct"; one can then evaluate again, correct again, and so on until one decides to move on from t_n to t_{n+1} . Since we are assuming f to be complicated, the cost of correcting is negligible and we therefore finish with an application of the corrector before moving to the next value of t. In an obvious notation we can denote the procedure, for a particular pair of predictor-corrector formulas, by $P(EC)^m$, where the number of iterations is $m = 1, 2, 3, \cdots$. We assume that m is the same for each step.

We want to study the way in which the relationship between accuracy and cost depends on the choice of predictor-corrector formulas and on the choice of m. To this end we first derive an expression for the propagated error, which will indicate how this error depends on the various factors involved.

Truncation errors and roundoff errors are defined in the following way. T_n^* , the truncation error in the predictor formula, is defined by

$$x_{n} = \sum a_{i}^{*} x_{n-i} + h \sum b_{i}^{*} x_{n-i}' + T_{n}^{*}, \qquad (4)$$

while T_n , the truncation error in the corrector formula, is defined by

$$x_n = \sum a_i x_{n-i} + h \sum b_i x'_{n-i} + T_n .$$
 (5)

Let $z_{n,j}$ denote the rounded result obtained from the *j*th application of the corrector formula at t_n , and let $z'_{n,j} = f(t_n, z_{n,j})$. It is convenient to let $z_{n,0}$ denote the rounded result obtained from the predictor at t_n . Then r_n^* , the roundoff error in the predictor, is defined by

$$z_{n,0} = \sum a_i^* z_{n-i,m} + h \sum b_i^* z_{n-i,m-1}' - r_n^*, \qquad (6)$$

while $r_{n,j}$, the roundoff error in the *j*th application of the corrector, is defined by

$$z_{n,j} = \sum a_{i} z_{n-i,m} + h b_{0} z'_{n,j-1} + h \sum_{i \neq 0} b_{i} z'_{n-i,m-1} - r_{n,j}.$$
(7)

Denote the propagated error by $e_n = x_n - z_{n,m}$, and define g through the equation f(t, u) - f(t, v) = g(u - v), so that g can usually be taken to be some value of $\partial f/\partial x$.

The error equations are obtained by subtracting (6) from (4), and each of equations (7) from (5). Of course these equations cannot be solved for e_n . However, we would like to obtain an expression which approximates e_n , at least to the extent that it indicates how e_n depends on the various factors involved in the procedure.

The argument is tedious but straightforward. First, substitute the constants r^* , r, T^* , T, and g into the error equations in place of the corresponding variable quantities. The error equations then become m+1 linear difference equations with constant coefficients. (The m+1 unknowns are $x_n - z_{n,j}$ for $j = 0, 1 \cdots$, m, but we are interested only in the propagated error, which is the unknown corresponding to j = m.)

The solutions of these difference equations depend on the zeros of a certain polynomial. As $m \to \infty$, the polynomial becomes $C(s) = s^k - \sum (a_i + hgb_i)s^{k-i}$, which is associated with the corrector alone. Even this special case is quite difficult, but it has received some study, for example in [2]. The polynomials of practical interest are those associated with correctors having $T = O(h^p)$, as $h \to 0$, for moderately large p. (Later we consider p = k + 2.) One zero of C(s) is then exp $(hg) + O(h^p)$, while the other k-1 extraneous zeros will cause instability unless their magnitudes are less than 1, or less than e^{hg} , depending on whether the stability is required to be absolute or relative.

When m is not large the polynomial is more complicated. It turns out to be

$$s^{k}C(s) + \theta^{m-1} \{ C(s) \sum_{i \neq 0} (b_{i} - b_{i}^{*} + \theta b_{i}^{*}) s^{k-i} + hg(\sum b_{i}s^{k-i}) \sum_{i \neq 0} (a_{i} - a_{i}^{*} + \theta a_{i}^{*} + hg(b_{i} - b_{i}^{*} + \theta b_{i}^{*})) s^{k-i} \},$$
(8)

where we have put $\theta = hgb_0$. As $m \to \infty$, k roots of this polynomial will approach 0. The other k roots will approach the roots of the preceding polynomial, one being associated with exp (hg), while the others are associated with the extraneous roots.

Later on we will return to questions regarding the stability of these predictorcorrector procedures. For the present, let us assume that they are stable. We also neglect the effect of starting errors. We then obtain the following expression for the propagated error.

$$e_{n} = \left\{ \frac{r+T}{hg\sum b_{i}} \left(1 - \frac{\theta^{m-1}(1-\theta)hg\sum b_{i}^{*}}{1-\theta^{m}} \right) + (r^{*}+T^{*})\frac{\theta^{m-1}(1-\theta)}{1-\theta^{m}} \right\} \{s_{1}^{n}-1\} + \{\text{small terms}\},$$
(9)

where s_1 is the zero of (8) which approaches $\exp(hg) + O(h^v)$ as $m \to \infty$. Thus, for large m, $s_1^n \approx \exp(g(t_n - t_0))$. (We have assumed $\theta \neq 1$, but, for convergence of the iterations, we in fact must assume much more, namely that $|\theta| < 1$.)

The expression in (9) indicates how the propagated error depends on the choice of procedure, as long as the procedure is stable. Before drawing any conclusions from this expression we should know a little more about the nature of T^* and T. If T^* and T are to be $O(h^p)$ for the same p, it is known that in general p cannot exceed k + 2, as long as the procedure is required to be stable. On the other hand, there is a wide choice of stable methods for which p = k + 2. Since it is obviously desirable to have p large, we will assume that p = k + 2. Then

$$T^* = R^* h^{k+2} + O(h^{k+3})$$
 and $T = R h^{k+2} + O(h^{k+3})$,

where R^* depends on the choice of a_i^* , and R depends on the choice of a_i .

Let us suppose that these expressions for T^* and T are substituted into (9). Then the propagated error is expressed in terms of the coefficients in the predictor-corrector formulas, along with h, g and m, as well as the number of steps n. We have already referred to an earlier paper [2] which was concerned with the special case obtained by letting $m \to \infty$. There the emphasis was on trying to choose stable procedures which minimized the factor $R/\sum b_i$. In the more general context of this paper it is more important to consider first the relative importance of the contributions from the corrector and the predictor.

We need consider only those situations in which T^* and T are more important than r^* and r, respectively. Otherwise we would consider a larger value of h. (This shows very clearly in the experimental results described in Section 3.)

We now show that it is then best to have m = 1 in (9). Note that the effect of a larger value of m is to reduce the contribution, in (9), of the predictor, i.e. of the term containing T^* . On the other hand, according to our assumption about f being complicated, it costs as much to increase the number of iterations as it does to decrease h by the same factor. There are two possibilities, and in either case it is better to reduce h than to increase m The first possibility is that $hg \sum b_i$ is so small that the term containing T dominates. The effect of increasing m is then negligible. In this case the extra cost involved in increasing m is not worthwhile, and m = 1 is best. The second possibility is that the term containing T^* dominates. The effect of m iterations is, approximately, to reduce this term by the factor θ^{m-1} . For the same cost, one can keep m = 1 but change h so that this term is instead reduced by the factor m^{-k-2} . (The term containing T is also reduced, but by a factor m^{-k-1} .) Of course m cannot be very large, for then T would dominate and the situation of the first possibility would result. Also, θ cannot be very small, for then $hg \sum b_i$ would also probably be small, and again the first possibility would result. Thus, when T^* dominates, we have only to consider m not very large and θ not very small. Then θ^{m-1} will in general be greater than m^{-k-2} , and it is better to reduce h than it is to increase m. (A typical example in practice is one where $\theta = .1$, m = 2 and k = 4. Here $\theta^{m-1} =$.1 and $m^{-k-2} < .02$, and it is preferable to use m = 1, with h replaced by h/2.)

We conclude that for a given cost and for given predictor-corrector formulas, the smallest value of (9) will be obtained with m = 1. This means that the most efficient predictor-corrector procedures will be those involving only a single evaluation and a single correction per step, at least as long as the stability requirement is satisfied.

Stability is determined by the zeros of (8), but we have been unable to derive from (8) any worthwhile indication of the way in which stability might be affected by changing m. A detailed study of some special cases has been given recently by Chase [1] along with results for some related procedures. But for the general case considered here we have to depend on experimental evidence to determine whether or not additional iterations can be justified in terms of the improvement in stability they might bring. Such evidence is described in the next section, along with the evidence for determining which formulas to use.

Before concluding this section we should mention that we have also investigated procedures which finish each step with an evaluation rather than a correction. (They can be denoted by $PE(CE)^m$, with $m = 0, 1, 2, \cdots$.) They are not of interest when f is complicated, but they could be in other contexts. Their error equations are simpler, and so is their fundamental polynomial, which turns out to be

$$C(s) + \theta^{m} \sum_{i \neq 0} (a_{i} - a_{i}^{*} + \theta a_{i} + hg(b_{i} - b_{i}^{*} + \theta b_{i}^{*}))s^{k-i}.$$
 (10)

Because (10) is simpler than (8), it is possible that one could derive something worthwhile from (10) about the way stability might be affected by changing m with this other class of procedures.

3. Experimental Results

For the experimental side of our investigation we first selected the predictorcorrector procedures which were to be tested. We decided to test procedures using formulas of the Adams type. These formulas are defined by taking $a_i^* = a_i = 1$, but otherwise $a_i^* = a_i = 0$, and then "matching coefficients" in (2) and (3) to obtain the b_i^* and b_i . The resulting formulas have $T^* = O(h^{k+2})$ and $T = O(h^{k+2})$.

We tested procedures for $k = 1, 2, \dots, 8$, and for each value of k we tried m = 1, 2, 3, 4.

We decided to consider only formulas of the Adams type because we believe

that other formulas cannot be significantly better, at least as long as we insist on considering only general-purpose procedures, as we do in this paper. Our belief is based primarily on the results of an earlier paper [2], where a representative collection of corrector formulas was tested for each value of k up to k = 8. For each value of k, the smallest error observed was rarely less than about a fifth of the error observed with Adams' formula. In exceptional cases the smallest error was better than this by another factor of about 10, but these cases were always associated with methods which were in other cases unstable. For example, Newton-Cotes formulas are especially good when g > 0 (and k is even), but they are unstable when g < 0. Thus they cannot be used for general-purpose procedures.

For a given value of k we therefore cannot, in general, find a corrector formula which is very much better than the Adams formula. Moreover, the Adams formula of step-number k + 1 or k + 2 was usually better than the best formula of step-number k.

On the basis of these results for corrector formulas, we decided to use only the predictor and corrector formulas of the Adams type. In any event we believed that these formulas were at least adequate, in the sense that the results obtained with them would be representative of what we could expect with different values of k and different values of m.

We tried each procedure on a total of 17 different differential equations. With each equation we used the procedure associated with each pair of values of k and m, with $h = 2^{-1}, 2^{-2}, \dots, 2^{-7}$. Each run was from t = 0 to t = 40. At t = 10, 20, 30, 40 the maximum error observed in the preceding interval of length 10 was shown. Additional runs were made for intermediate values of h to provide more detail in some of the resulting graphs. In each case the true solution was used to provide the starting values.

We describe in detail the results for one problem which was representative of most of the others. We then refer more briefly to the results for the other problems, especially to those which showed the greatest variations from the first one.

The first problem is defined by

(A),
$$x' = -x + 10 \sin 3t$$
, with the solution $x = \sin 3t - 3 \cos 3t$,

and we consider results obtained for the interval $0 < t \leq 40$.

Figure 1 is typical of the curves we shall be considering. It shows the relationship between accuracy and cost when the Adams procedure with k = 4 and m = 1 is used on problem (A). The curve is dotted in the instability region because it is only a bound for the error in this region; not surprisingly, we often found errors which were quite unpredictable in the small region of transition between stability and overflow. The curve also behaves as one would expect in the region of stability in that it at first decreases as h decreases, but eventually increases as h decreases still further. These latter changes show first the influence of truncation error, and then of roundoff error.

The curve of Figure 1 appears again in Figure 2, where it is compared with the

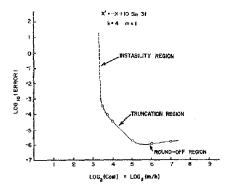


FIG. 1. Variation of accuracy with cost for a typical procedure. The largest absolute error, for $0 < t \leq 40$, is denoted by [ERROR].

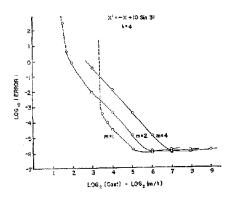


FIG. 2. Accuracy-cost curves showing the effect of changing the number of iterations. The procedure with m = 1 is best, as long as it is stable.

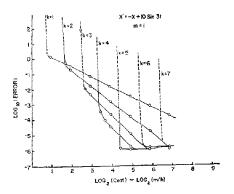


FIG. 4. Results for problem (A), using procedures with $m \approx 1$. They are not quite as good as the results using $m \approx 2$ (see Fig. 5).

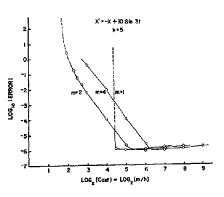


FIG. 3. An extra iteration to ensure stability (m=2) is more likely to be needed when k is large. Compare these results (k=5) with Fig. 2 (k=4).

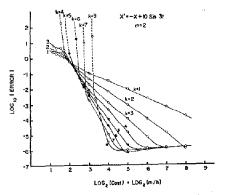


FIG. 5. Results for problem (A), using procedures with m = 2. They are slightly better than the results using m = 1 (see Fig. 4).

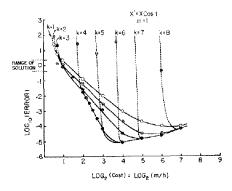


FIG. 6. Problem (E), using m = 1. Slightly better than using m = 2 (Fig. 7).

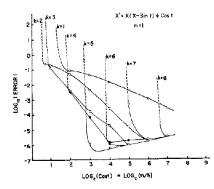


FIG. 8. Problem (H), using m = 1. Comparable to results using m = 2 (Fig. 9).

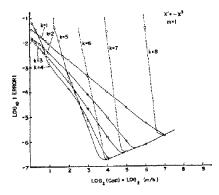


FIG. 10. Problem (K), using m=1. Not nearly as good as using m=2 (Fig. 11).

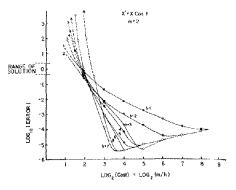


FIG. 7. Problem (E), using m = 2. Not quite as good as using m = 1 (Fig. 6).

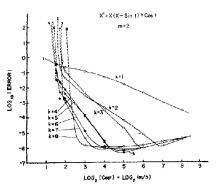


FIG. 9. Problem (H), using m = 2. Comparable to results using m = 1 (Fig. 8).

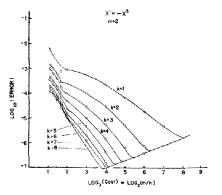


FIG. 11. Problem (K), using m = 2. Much better than using m = 1 (Fig. 10).

curves for procedures using the same formulas but with different numbers of iterations. It is clear that m = 1 is best as long as the corresponding procedure is stable, as was expected. However, m = 2 is best in a small region where the procedure for m = 1 is unstable; the step-size h and the error are both relatively large in this region.

The better stability associated with m = 2, compared to m = 1, is even more pronounced with larger values of k. This is illustrated in Figure 3, where the corresponding results are given for k = 5.

In none of the examples tried was m = 3 or m = 4 superior to m = 2. We were left with having to decide between m = 1 and m = 2. To make such a decision we compared all the curves for m = 1 $(k = 1, 2, \dots 8)$ with the corresponding curves for m = 2.

Figure 4 gives the curves obtained for problem (A) when m = 1, while Figure 5 gives the results when m = 2. The best that one can do with m = 1 is represented in Figure 4 by the lower left edge of the collection of curves shown there, while the best one can do with m = 2 is represented by the corresponding edge of the curves shown in Figure 5.

The edge for m = 2 is slightly better than the edge for m = 1, over the range of error that would be of interest. On the basis of this comparison we would therefore choose m = 2 in preference to m = 1. Moreover, there is an additional advantage with m = 2 which appears here, as well as in the later examples. It is clear that the best value of k in each case depends on the error, and will increase if we make the accuracy requirements more stringent. However, the best value of k is more sensitive to the accuracy requirement when m = 1 than when m = 2. In practice it would be very difficult to choose the appropriate value of k when m = 1, but when m = 2 a single value of k gives a method whose results are nearly as good as those along the critical edge. A value of 6 or 7 for k will do almost as well as the best, over practically all of the range of error which would ordinarily be considered tolerable.

Three other problems were much like problem (A), leading to similar results. They were

- (B) $x' = -x + 2 \sin t$, with $x = \sin t \cos t$,
- (C) $x' = x + 2 \sin t$, with $x = -\sin t \cos t$,
- (D) $x' = -3x + 10 \sin t$, with $x = 3 \sin t \cos t$.

In the remaining problems we found some in which m = 1 was slightly better than m = 2, others in which the two were about equally good, and one in which m = 2 was much better. We offer very briefly some examples which illustrate these possibilities. They will turn out to be sufficiently consistent that quite definite conclusions can be drawn from them.

In the following three problems, m = 1 was slightly better than m = 2.

- (E) $x' = x \cos t$, with $x = \exp(\sin t)$,
- (F) $x' = x \cos^2 t$, with $x = \exp(\frac{1}{2}t + \frac{1}{4}\sin 2t)$,
- (G) $x' = (x \sin t) \log(1 + t/40) + \cos t$, with $x = \sin t$.

Figures 6 and 7 give the results for problem (E), with the interval $0 < t \leq 40$. In the following three problems, the two values of *m* were about equally good.

- (H) $x' = x(x \sin t) + \cos t$, with $x = \sin t$,
- (I) $x' = x(x \sin^2 t) + \sin 2t$, with $x = \sin^2 t$,
- (J) x' = -tx/(4t + 16), with $x = (t + 4)\exp(-t/4)$.

Figures 8 and 9 give the results for problem (H), with the interval $0 < t \leq 40$.

In one problem the results for m = 2 were much better than those for m = 1. The problem is the following:

(K)
$$x' = -x^3$$
, with $x = (2t + 2)^{-1/2}$.

The results are presented in Figures 10 and 11, for the interval $0 < t \leq 40$.

The results of the remaining six problems were almost completely dominated by roundoff, and so no useful comparison could be made. To obtain useful results with such problems it would be necessary to try larger values of h, over longer intervals. The following problems were of this type:

(L)
$$x' = x/4$$
, with $x = \exp(t/4)$
(M) $x' = x - 2t/x$, with $x = (2t + 1)^{1/2}$
(N) $x' = x/40$, with $x = \exp(t/40)$
(O) $x' = x^2$, with $x = (40.01 - t)^{-1}$
(P) $x' = x^{1/2}$, with $x = (5 + t/2)^2$
(Q) $x' = (1 + x^2)/2(2500 - t^2)^{1/2}$, with $x = ((50 + t)/(50 - t))^{1/2}$.

Before considering the conclusions to be drawn from these results we would like to remark on two special features which occasionally appeared. One was a dip in the curve which sometimes occurred immediately to the right of where instability had caused overflow. We attributed this to a change of sign, at that point, in the error of largest magnitude. The other special feature was a dip in the curve to a point below the "roundoff line" which sometimes appeared between the truncation region and the roundoff region. (A mild example of this appears on the curve for k = 3 in Figure 7.) We attributed this to the bias which existed in the rounding procedures, which could in turn cause the roundoff error to favor one sign, so that the accumulated effect of roundoff could tend to compensate for the effect of truncation error, when the latter was of opposite sign and when both errors were of about the same magnitude.

4. Conclusions

Our purpose has been to study the efficiency of predictor-corrector procedures with a view to deciding which procedures should be used in practice.

We have considered the total number of evaluations of f, and hence m/h, to be a measure of the cost, and this corresponds to the case where f is fairly complicated. We have also restricted our interest to procedures which can be generalpurpose, and this has led us to consider only those of the Adams type.

We have concentrated our attention on the relationship between accuracy and cost, and we have been concerned with how this relationship depends on the procedure being used, that is, on the step-number k and the number of iterations m.

We have observed that two effects take place when k is increased. One is that the truncation region is lowered. Unfortunately this desirable effect is at

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least partially offset by the other one, which is that the region of instability moves to the right.

On the other hand, opposite effects take place when m is increased while k is held fixed. The truncation region is raised, and the instability region is moved to the left. Our theory had led us to expect the first of these effects, but we had been unable to decide theoretically about the second.

Experimental results are needed to determine the net effect of all these competing factors. The results for quite a variety of different differential equations are consistent enough that we are able to draw some definite conclusions.

One conclusion is that m = 2 is best. On the average it seems to be slightly better than m = 1, while m = 3 and m = 4 are not worth considering. Moreover, with m = 2 there is at least one value of k which will do well over most of the error range that is of interest, whereas with m = 1 different values of k would have to be determined for different parts of that range.

One other advantage of m = 2 compared to m = 1 is that one is able, with m = 2, to obtain a measure of the size of g at each step in the calculation. This means that one is able to have automatic stability control during the course of a calculation, as well as the usual automatic error control. This possibility has already been considered by Nordsieck [3], who has considered in great detail a procedure corresponding to the Adams procedure with k = 5 and m = 2.

In summary, it appears that the best predictor-corrector procedures, at least for general purposes, assuming f is fairly complicated, are those which involve two evaluations of f and two applications of the corrector formula per step. Such procedures are at least as accurate as any others on the average, and moreover they have additional advantages in the ease with which one can choose the step-number k and monitor the stability. It appears that the extra iteration is needed for the sake of stability.

On the other hand, it also appears that relatively large values of k are needed to provide sufficient accuracy. In our examples, both of the values k = 6 and k = 7 were good over adequately wide ranges of error. Of course, in practice these procedures should be used only with both error and stability control. Stability control would be especially necessary in view of the high step-numbers involved.

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