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Exponential Fitting of Matricial Multistep Methods for Ordinary Differential Equations

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Abstract. We study a class of explicit or implicit multistep integration formulas for solving $N \times N$ systems of ordinary differential equations. The coefficients of these formulas are diagonal matrices of order N, depending on a diagonal matrix of parameters Q of the same order. By definition, the formulas considered here are exact with respect to $y' = -Dy + \phi(x, y)$ provided $Q = hD$, h is the integration step, and ϕ belongs to a certain class of polynomials in the independent variable x. For arbitrary step number $k \geqslant 1$, the coefficients of the formulas are given explicitly as functions of Q. The present formulas are generalizations of the Adams methods ($Q = 0$) and of the backward differentiation formulas ($Q = +\infty$). For arbitrary Q they are fitted exponentially at Q in a matricial sense. The implicit formulas are unconditionally fixed-h stable. We give two different algorithmic implementations of the methods in question. The first is based on implicit formulas alone and utilizes the Newton-Raphson method; it is well suited for stiff problems. The second implementation is a predictor-corrector approach. An error analysis is carried out for arbitrarily large Q. Finally, results of numerical test calculations are presented.

1. Introduction. This paper is concerned with a class of integration formulas for $N \times N$ systems of ordinary differential equations proposed earlier by one of the authors [1]. These formulas are of linear multistep type,

$$\sum_{j=-(k-1)}^{1} \alpha_{j+k-1}(Q) y_{n+j} - h \sum_{j=-(k-1)}^{1} \beta_{j+k-1}(Q) y'_{n+j} = 0. \tag{1.1}$$

Their coefficients $\alpha_j(Q)$ and $\beta_j(Q)$ are diagonal matrices of order N depending on a diagonal matrix Q of parameters of the same order. By the symbol $\mathbf{F}_k$ we refer to the explicit ("predictor") k-step formula ($\beta_k = 0$) and by $\mathbf{F}_k^*$ to the implicit ("corrector") formula ($\beta_k \neq 0$) of the same length. Similarly, F_k and F_k^* denote generic scalar components (rows) of $\mathbf{F}_k$ and $\mathbf{F}_k^*$, respectively. By definition, $\mathbf{F}_k$ or $\mathbf{F}_k^*$ are exact, for arbitrary fixed Q, when applied to

$$y' = -Dy + \phi(x, y), \tag{1.2}$$

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with $Q = hD$, provided $\phi(x, y(x))$ is any polynomial in the independent variable x of degree $\leqslant k - 1$ or $\leqslant k$, respectively. Each row F_k or F_k^* depends solely on $q = hd$, where d and q are the corresponding diagonal entries of D and Q, respectively. Systems of the form (1.2) arise naturally in applications, e.g., in nuclear reactor calculations [2]. The approach taken in this paper is related to those of Cohen and Flatt [3] and of Guderley and Hsu [4].

Any $N \times N$ system

$$y' = f(x, y) \tag{1.3}$$

takes, of course, the form (1.2) if we let $\phi = Dy + f$. However, as one would expect, the formulas considered here lend themselves particularly well to problems in which ϕ is in some sense small compared to f or to Dy. Even so the present formulas remain meaningful and competitive with well-known conventional methods when parametrized by $\tilde{Q} = h\tilde{D}$, $\tilde{D} \neq D$, rather than by Q. In fact, for $q = 0$, F_k and F_k^* are simply the explicit and implicit k-step Adams formulas, respectively. Similarly, subject to appropriate scaling, F_k^* for $q = +\infty$ is the k-step backward differentiation formula (BDF). For arbitrary q, $0 \leqslant q \leqslant +\infty$, F_k^* is exponentially fitted [5] at $q = hd$. Nevertheless, a certain amount of caution is needed in fitting at locations $\tilde{Q} \neq Q$, as explained in the second-to-last paragraph of Section 3.

The formulas $\mathbf{F}_k^*$ are useful for integrating stiff [6] systems because, when fitted at large q's, the F_k^* possess some of the strong fixed-h stability properties required to control the corresponding "rapid transients". More specifically, F_1^* is A-stable [7] for any q, $0 \leqslant q \leqslant +\infty$. F_2^* is A-stable for any q, $2 < q \leqslant +\infty$. F_3^* is $A(\alpha)$-stable [8] and stiffly stable [9] for any $q \geqslant 5$. For arbitrary k, F_k^* is A_∞-stable [10] for any sufficiently large q. On the other hand, when fitted at sufficiently small values of $|q|$, F_k and F_k^* are stable [11] for arbitrary k and thus well suited for treating nonstiff components. More specifically, F_3^* is stable for all q, $0 \leqslant q \leqslant +\infty$.

If the implicit formula $\mathbf{F}_k^*$ is applied to (1.2) or (1.3), a set of algebraic equations, in general nonlinear, must be solved at every time step. It has been found [12] that, in dealing with stiff problems, the Newton-Raphson (NR) method is useful for accomplishing this task. The iteration can be started, e.g., from a first guess obtained by polynomial extrapolation from previous solution values.* With a sufficiently accurate first guess, only one or two NR steps need to be carried out to make the stopping error of the iteration compatible with the local truncation error [13]. The fixed-h

*Obviously, with large integration steps, this technique is meaningful primarily during the asymptotic phase of the solution; i.e., after the stiff components have been damped out. During the initial, transient phase, it is appropriate to use small integration steps to sample the rapidly varying solutions.

stability analysis of the formulas F_k^*, $k \geqslant 1$, given in this paper remains valid even when we use one single NR iteration step. The reason for it is that this analysis is carried out relative to a linear test equation [7],

$$y' = \lambda y, \qquad \lambda = \text{const}, \tag{1.4}$$

and that for linear equations the NR method converges in one step.

Some iterative methods of solving the difference equations other than the NR technique are sensitive to stiffness and in its presence become inefficient. This is the case, e.g., for the straight Picard iteration [12]. Similarly, as one can deduce from the results of [4], it is not recommendable to use finite predictor-corrector (PC) algorithms in solving stiff problems because, with such algorithms, the unconditional fixed-h stability properties of the F_k^* are lost [12]. This is, of course, due to the explicit character of such finite PC methods [7]. However, as mentioned in the last section of this paper, exponentially fitted, finite PC methods are useful for solving nonstiff problems with relatively large integration steps.

A class of parametrized multistep methods similar to the one considered here is described in [14]. Those methods have step number k and order of accuracy $p = 2k$, and are said to be A-stable. For $k \geqslant 1$ this contradicts the well-known constraint $p \leqslant 2$ for A-stability [7]. The discrepancy stems from the fact that in [14], as well as in [15], the term A-stability is, somewhat misleadingly, used to identify a much weaker stability property than in [7]. In its original spirit, this term was used relative to an integration formula with fixed coefficients, applied to the test equation (1.4) with arbitrary complex λ, $\operatorname{Re}\lambda < 0$. Similarly, in the present paper, fixed-h stability analysis is carried out for given fixed values of d or q, and thus fixed coefficients, but for an arbitrary complex λ which varies independently of d. As opposed to this, the term A-stability in [14] and [15] means fixed-h stability for any λ, $\operatorname{Re}\lambda < 0$, of a parametrized formula whose coefficients, for each λ, are exponentially fitted at λh. In other words, the results of [14] and [15] are restricted to the special case $d = \lambda$.

The outline of the present paper is as follows: In Section 2 we give explicit expressions for the coefficients of $\mathbf{F}_k$ and $\mathbf{F}_k^*$ for arbitrary k. We discuss the relationship between these formulas and Adams methods, BDF, and exponentially fitted formulas in the sense of [5]. In Section 3 we study unconditional fixed-h stability and stability of the formulas F_k^*. Section 4 is devoted to algorithmic aspects. We define a one-step Newton-Raphson implementation of $\mathbf{F}_3^*$. Then we analyze the local truncation error of the formulas $\mathbf{F}_k$ and $\mathbf{F}_k^*$. The result of this analysis is used to define PC algorithms. Finally, in Section 5, we describe numerical results obtained for various test problems. The performance of the methods considered here compares favorably with that of other existing methods.

2. Derivation of Integration Formulas. A. The analysis of parts A and B of this section is presented in more detail in [16]; it is similar to the one given in [17].

Let $\{x_n\}$, $x_n = nh$, $n = 0, 1, \cdots, h > 0$. Equation (1.2) can be converted into an integral equation,

$$y(x_{n+1}) = e^{-hD}y(x_n) + \int_{x_n}^{x_{n+1}} e^{-(x_{n+1}-x)D}\phi(x, y(x))\,dx, \tag{2.1}$$

where x_n is fixed, x_{n+1} represents the independent variable, and $h = x_{n+1} - x_n$. With (2.1) we can associate a class of linear multistep formulas. To do this we approximate $\phi(x, y)$ by a polynomial in x and evaluate the integral in closed form. If the polynomial is defined by Lagrange interpolation through $\phi_{n-i} = \phi(x_{n-i}, y_{n-i})$, $i = 0, 1, \cdots, k-1$, $k \geqslant 1$, this procedure results in a k-step formula $\mathbf{F}_k$ of explicit or predictor type. If, on the other hand, Lagrange interpolation through ϕ_{n-i+1}, $i = 0, \cdots, k$, is used, an implicit or corrector formula $\mathbf{F}_k^*$ with the same number of steps is obtained.

In order to derive $\mathbf{F}_k$, we use Newton's backward difference formula [18] to fit a polynomial $\hat{\phi}(x)$ through ϕ_{n-i}, $i = 0, \cdots, k-1$. If in (2.1) we replace ϕ by $\hat{\phi}$ we obtain the difference form of $\mathbf{F}_k$,

$$y_{n+1} - e^{-Q}y_n - h\sum_{i=0}^{k-1} G_i\nabla^i\phi_n = 0, \qquad k \geqslant 1, \tag{2.2}$$

where ∇^i denotes the ith backward difference, $Q = hD$, and

$$G_i = (-1)^i \int_0^1 e^{-(1-\xi)Q}\binom{-\xi}{i}d\xi, \qquad i = 0, 1, \cdots. \tag{2.3}$$

Upon evaluation of the integral [19] this yields

$$G_i = \sum_{j=0}^{i} \psi_{ij}Q^{-(j+1)} - e^{-Q}\sum_{j=0}^{i} \xi_{ij}Q^{-(j+1)}, \qquad i \geqslant 0, \tag{2.4}$$

where

$$\psi_{ij} = \frac{j!}{i!}\,\gamma_{ij}, \qquad i \geqslant 0,\ 0 \leqslant j \leqslant i, \tag{2.5}$$

$$\xi_{ij} = \frac{1}{i!}\sum_{l=j}^{i} \gamma_{il}\,l!/(l-j)!, \qquad 0 \leqslant j \leqslant i, \tag{2.6}$$

and where the γ_{ij}, $i \geqslant 0$, $0 \leqslant j \leqslant i$, are defined by

$$\binom{-\xi}{i} \equiv \frac{(-1)^i}{i!}\sum_{j=0}^{i} \gamma_{ij}\zeta^j, \qquad i \geqslant 0, \tag{2.7}$$

with $\zeta = 1 - \xi$. Obviously, $\gamma_{0,0} = \gamma_{1,0} = 1$ and $\gamma_{1,1} = -1$. It is easy to show that the γ_{ij} satisfy the recurrence relations

$$\left.\begin{aligned} \gamma_{i+1,0} &= (i+1)\gamma_{i,0}, \\ \gamma_{i+1,i+1} &= -\gamma_{ii}, \\ \gamma_{i+1,j} &= (i+1)\gamma_{ij} - \gamma_{i,j-1}, \qquad 1 \leqslant j \leqslant i \end{aligned}\right\}, \qquad i \geqslant 1. \tag{2.8}$$

Note that

$$\sum_{j=0}^{i} \gamma_{ij} = 0, \qquad i \geqslant 1, \tag{2.9}$$

which follows from (2.7) for $\zeta = 1$. From (2.9) it follows that $\xi_{i,0} = 0, i > 1$.

To transform $\mathbf{F}_k$ into ordinate form, we make the substitution

$$\nabla^i \phi_n = \sum_{j=0}^{i} (-1)^i \binom{i}{j} \phi_{n-j}, \qquad i = 0, 1, \cdots.$$

This yields

$$y_{n+1} - e^{-Q} y_n - h \sum_{i=0}^{k-1} B_{k-1,i} \phi_{n-i} = 0, \qquad k \geqslant 1, \tag{2.10}$$

where

$$\begin{aligned} B_{ij} &= (-1)^j \sum_{l=j}^{i} \binom{l}{j} G_l \\ &= \sum_{l=0}^{i} \mu_{ijl} Q^{-(l+1)} - e^{-Q} \sum_{l=0}^{i} \nu_{ijl} Q^{-(l+1)}, \qquad i \geqslant 0,\ 0 \leqslant j \leqslant i, \end{aligned} \tag{2.11}$$

and where

$$\begin{Bmatrix} \mu \\ \nu \end{Bmatrix}_{ijl} = (-1)^j \sum_{r=\max(j,l)}^{i} \binom{r}{j} \begin{Bmatrix} \psi \\ \xi \end{Bmatrix}_{rl}, \qquad 0 \leqslant j \leqslant i,\ 0 \leqslant l \leqslant i, \tag{2.12}$$

meaning that μ and ν are associated with ψ and ξ, respectively.

B. An analysis very similar to the one given above for the formulas $\mathbf{F}_k$ can be carried out for the $\mathbf{F}_k^*$. All quantities associated with these implicit formulas are so identified by asterisks. The difference form of $\mathbf{F}_k^*$ is

$$y_{n+1} - e^{-Q} y_n - h \sum_{i=0}^{k} G_i^* \nabla^i \phi_{n+1} = 0, \qquad k \geqslant 1, \tag{2.13}$$

where

$$\begin{aligned} G_i^* &= (-1)^i \int_{-1}^{0} e^{\xi Q} \binom{-\xi}{i} d\xi \\ &= \sum_{j=0}^{i} \psi_{ij}^* Q^{-(j+1)} - e^{-Q} \sum_{j=0}^{i} \xi_{ij}^* Q^{-(j+1)}, \qquad i = 0, 1, \cdots. \end{aligned} \tag{2.14}$$

Here

$$\left.\begin{aligned} \psi_{ij}^* &= (-1)^j \frac{j!}{i!} \gamma_{ij}^* \\ \xi_{ij}^* &= \frac{1}{i!} \sum_{l=j}^{i} (-1)^l \gamma_{il}^* \frac{l!}{(l-j)!} \end{aligned}\right\}, \qquad 0 \leqslant j \leqslant i, \tag{2.15}$$

and it is easy to show that the quantities γ_{ij}^*, which are defined by the relation

$$\binom{-\xi}{i} \equiv \frac{(-1)^i}{i!} \sum_{j=0}^{i} \gamma_{ij}^* \xi^j, \qquad i \geqslant 0, \tag{2.16}$$

satisfy $\gamma_{ij}^* = \xi_{ij}$ for all i, j. By definition, $\xi_{i,0}^* = 0$ for $i \geqslant 2$.

The relation (2.13) is equivalent to

$$y_{n+1} - e^{-Q} y_n - h \sum_{i=0}^{k} B_{ki}^* \phi_{n+1-i} = 0, \qquad k \geqslant 1, \tag{2.17}$$

the ordinate form of $\mathbf{F}_k^*$, where

$$B_{ij}^* = (-1)^j \sum_{l=j}^{i} \binom{l}{j} G_l^*, \qquad i \geqslant 0,\ 0 \leqslant j \leqslant i. \tag{2.18}$$

The relationship (2.18) between the B_{ij}^* and G_l^* is the same as that between the B_{ij} and G_l, respectively. The equations (2.11) and (2.12) thus remain valid between the "starred" quantities.

In the limit where a component q of Q tends to zero, the calculation by the closed expressions given in this section, of the components $g_i(q)$ and $g_i^*(q)$ of $G_i(Q)$ and $G_i^*(Q)$, respectively, is affected by roundoff errors. In this limit it is preferable to compute the quantities g_i and g_i^* by power series expansions as mentioned in Section 4 below.

C. The formulas considered in this paper are generalizations of conventional Adams formulas. More specifically, in the limit $q \to 0$, F_k or F_k^* tend to the explicit or implicit k-step scalar Adams formula, respectively. In fact, it is shown in Section 4 that, if q is treated as an independent, constant parameter, the local truncation error of F_k^* is $q g_{k+1}^* h^{k+1} y_n^{(k+1)} + O(h^{k+2})$. Therefore, for $q = 0$, the order of accuracy [20] of F_k^* is $p = k + 1$. Also, for $q = 0$, we have $\phi = y'$ according to (1.2) and thus F_k^* is of Adams type; i.e., it involves the two leading terms only of y. Because of uniqueness [21], this formula is, in fact, the well-known k-step implicit Adams formula. A similar argument shows that, for $q = 0$, the formula F_k is the explicit k-step Adams formula of order $p = k$.

Now consider the limit $q \to +\infty$. Here, if we neglect exponentially small terms versus negative powers of q, we find that $g_0^* = \psi_{0,0}^* q^{-1} = q^{-1}$ and $g_i^* = \psi_{i,1}^* q^{-2} + O(q^{-3})$, $i \geqslant 1$. Therefore, if we let

$$\theta_{k,0}^* = \sum_{i=1}^{k} \psi_{l,1}^*,$$

$$\theta_{kj}^* = (-1)^j \sum_{l=j}^{k} \binom{l}{j} \psi_{l,1}^*, \qquad 1 \leqslant j \leqslant k,$$

and if by b_{kj}^* we denote a generic diagonal component of B_{kj}^*, we have

$$b_{k,0}^* = q^{-1} + \theta_{k,0}^* q^{-2} + O(q^{-3}),$$

$$b_{kj}^* = \theta_{kj}^* q^{-2} + O(q^{-3}), \qquad 1 \leqslant j \leqslant k.$$

Thus, since $h\phi_{n+1-j} = hy'_{n+1-j} + qy_{n+1-j}$, one finds

$$b^*_{k,0}h\phi_{n+1} = y_{n+1} + \theta^*_{k,0}q^{-1}y_{n+1} + hq^{-1}y'_{n+1} + O(q^{-2}),$$
$$b^*_{kj}h\phi_{n+1-j} = \theta^*_{kj}q^{-1}y_{n+1-j} + O(q^{-2}), \qquad 1 \leqslant j \leqslant k,$$

and, after multiplying the formula F^*_k through by q, this formula, in the limit $q \to +\infty$, becomes

$$\sum_{j=0}^{k} \alpha_{k-j}y_{n+1-j} - hy'_{n+1} = 0, \tag{2.19}$$

where the coefficients α_i, $i = 0, \cdots, k$, depend of course on k. Formula (2.19) is of BDF type; i.e., it contains only one single y'-term, the leading one. But for any $q \neq 0$ the truncation error of F^*_k given above is $O(h^{k+1})$, i.e., F^*_k has order $p = k$. Again by uniqueness [21], the formula (2.19) is thus identical with the standard k-step BDF, normalized to $\beta_k = 1$.

Finally, by a similar argument as in the case $q \to +\infty$, one concludes that for any q, $0 < q < +\infty$, the component formula F^*_k is identical with the general k-step formula fitted exponentially at q in the sense of [5].

3. Stability Analysis. In proving A-stability [7] for linear multistep formulas we may, according to [22], test the two sufficient conditions N1: $|\sigma_i| < 1$, $i = 1, \cdots, k$, where σ_i are the roots of $\sigma(w)$, and N2: $\mathrm{Re}[\rho(w)/\sigma(w)] \geqslant 0$ for all w, $|w| = 1$. Via the transformations $w = w(z) = (z+1)/(z-1)$, $r(z) = (z-1)^k\rho(w(z))$, and $s(z) = (z-1)^k\sigma(w(z))$, condition N1 takes the form N1′: $\mathrm{Re}\, s_i < 0$, $i = 1, \cdots, k$, where the s_i are the roots of $s(z)$. N1′ can be tested by the Routh-Hurwitz theory [23]. One writes $s(z) = a_0z^k + b_0z^{k-1} + a_1z^{k-2} + \cdots$ and denotes by $a_0, b_0, c_0, \cdots$ the entries of the first column of the Routh tableau. Then N1′ is satisfied if and only if $a_0, b_0, c_0, \cdots$ are all nonzero and of equal sign. In discussing fixed-h stability with respect to the test equation (1.4) we use the notation $q' = \lambda h$, as distinguished from the fitting location, $q = dh$ (see second-to-last paragraph of Introduction).

The formula

$$F^*_1: -y_n + y_{n+1} - h\{[q^{-1} - (e^q - 1)^{-1}]y'_n + [(1 - q^{-1}) + (e^q - 1)^{-1}]y'_{n+1}\} = 0 \tag{3.1}$$

is A-stable for any q, $0 \leqslant q \leqslant +\infty$. In fact, as is shown in [12], the exponentially fitted, weighted Euler formula possesses this property and, according to the previous section, the latter and F^*_1 are equivalent.

In [5] it is stated without proof that, for $2 < q \leqslant +\infty$, the exponentially fitted two-step formula of order $p = 2$, which is equivalent to

$$
\begin{aligned}
F_2^*:\ & [(1-2q^{-1})+e^{-q}(1+2q^{-1})]\,y_{n-1}+4[(-1+q^{-1})-e^{-q}q^{-1}]\,y_n \\
& +[(3-2q^{-1})+e^{-q}(-1+2q^{-1})]\,y_{n+1} \\
& -h\{[(-q^{-1}+2q^{-2})-e^{-q}(q^{-1}+2q^{-2})]\,y'_{n-1} \\
& \quad +[(4q^{-1}-4q^{-2})-e^{-q}(2-4q^{-2})]\,y'_n \\
& \quad +[(2-3q^{-1}+2q^{-2})-e^{-q}(-q^{-1}+2q^{-2})]\,y'_{n+1}\} = 0
\end{aligned} \tag{3.2}
$$

is A-stable. Here we give a proof: We find ** $a_0 = g_0^* = [(1-e^{-q})/q] > 0$, $q > 0$. Let $\hat{b}_0 = q^2 b_0/2 = q-(1-e^{-q})$, where $b_0 = 2(g_0^* + g_1^*)$. Then $\hat{b}'_0(q) > 0$, $q > 0$, and $\hat{b}_0(0) = 0$. Thus $\hat{b}_0(q) > 0, q > 0 \Rightarrow b_0(q) > 0, q > 0$. Finally, let $\hat{c}_0 = q^3 c_0 = (2-q)\,[(2-q)-(2+q)e^{-q}]$, where $c_0 = a_1 = g_0^* + 2g_1^* + 4g_2^*$. We have $[\ ] < 2-q \leqslant 0$, $q \geqslant 2$, and thus $\hat{c}_0 > 0$, $q > 2$, which implies $c_0 > 0$, $q > 2$. Therefore N1′ is satisfied for $q > 2$. Condition N2 requires that $P(\xi, q) = 2\gamma(q)\,(\xi-1)^2 \geqslant 0$, $-1 \leqslant \xi \leqslant 1$, where

$$
\gamma(q) = q^{-5}\gamma_1(q)\gamma_2(q), \qquad \gamma_1(q) = \tfrac{1}{2}\,[(2-q)-(2+q)e^{-q}],
$$
$$
\gamma_2(q) = (-2+3q-q^2)+(2-q)e^{-q}.
$$

As stated above, $\gamma_1(q) > 0$ for $q > 2$. But $\gamma_2(q) < -q^2+3q-2 = (q-2)(1-q) < 0$, $q > 2$; thus $\gamma(q) > 0$, $q > 2$, and $P(\xi, q) \geqslant 0$ for all ξ, $-1 \leqslant \xi \leqslant 1$, $q > 2$, which completes the proof of A-stability.

The formula

$$
\begin{aligned}
F_3^*:\ & [(11-12q^{-1}+6q^{-2})-e^{-q}(2-6q^{-1}+6q^{-2})]\,y_{n+1} \\
& +[(-18+30q^{-1}-18q^{-2})-e^{-q}(3+12q^{-1}-18q^{-2})]\,y_n \\
& +[(9-24q^{-1}+18q^{-2})-e^{-q}(-6-6q^{-1}+18q^{-2})]\,y_{n-1} \\
& +[(-2+6q^{-1}-6q^{-2})-e^{-q}(1-6q^{-2})]\,y_{n-2} \\
& -h\{[(6-11q^{-1}+12q^{-2}-6q^{-3})-e^{-q}(-2q^{-1}+6q^{-2}-6q^{-3})]\,y'_{n+1} \\
& \quad +[(18q^{-1}-30q^{-2}+18q^{-3})-e^{-q}(6-3q^{-1}-12q^{-2}+18q^{-3})]\,y'_n \\
& \quad +[(-9q^{-1}+24q^{-2}-18q^{-3})-e^{-q}(6q^{-1}+6q^{-2}-18q^{-3})]\,y'_{n-1} \\
& \quad +[(2q^{-1}-6q^{-2}+6q^{-3})-e^{-q}(-q^{-1}+6q^{-3})]\,y'_{n-2}\} = 0
\end{aligned} \tag{3.3}
$$

is A_∞-stable [10] (i.e., N1′ is satisfied) for $q \geqslant 5$. To prove it we show that a_0, b_0, $c_0 = a_1 - (a_0 b_1/b_0)$, and $d_0 = b_1$ are nonzero and of equal sign for $q \geqslant 5$. First $a_0 = 6(1-e^{-q}) > 0$ for any $q > 0$. Then

$$
b_0 = (18-12q^{-1})+(-6+12q^{-1})e^{-q} \geqslant (18-12q^{-1})+(-6+12q^{-1}) = 12 > 0
$$

** By g_i and g_i^* we denote generic diagonal entries of G_i and G_i^*, respectively.

for $q \geq 2$. Next write $d_0 = 2q^{-3}[p_1(q) + p_2(q)e^{-q}]$. One finds $p_2'(q) > 0$ for $q \geq 2$, $p_2(2) > 0$, and thus $p_2(q) > 0$, $q \geq 2$. Similarly, $p_1'(q) > 0$, $q \geq 4$; $p_1(5) > 0$, and thus $p_1(q) > 0$ and $d_0 > 0$ for all $q \geq 5$. Finally subject to condition $b_0 > 0$ which is satisfied for $q \geq 2$, we have

$$c_0 > 0 \Longleftrightarrow a_1 b_0 - a_0 b_1 = q^2 N(q)/48 > 0,$$

where

$$N(q) = (6q^2 - 13q + 9) + (8q - 12)e^{-q} - (q - 3)e^{-2q}.$$

For $q > 3$, $8q - 12 > 0$ and $q - 3 > 0$. Hence,

$$N(q) > (6q^2 - 13q + 9) - (q - 3) = 6q^2 - 14q + 12 > 0$$

for all $q \geq 5$, which completes the proof that F_3^* is A_∞-stable for $q \geq 5$.

For $q \geq 5$, F_3^* possesses other properties of strong fixed-h stability, as a numerical investigation of the relevant conditions showed. In particular it was found that F_3^* is $A(\alpha)$-stable [8] for $\alpha \leq \alpha_0(q)$. The maximum angle $\alpha_0(q)$ increases from $\approx 84.4^\circ$ (1.4731 in radians) for $q = 5$ to $\approx 86^\circ$ for $q = +\infty$, the latter representing the three-step BDF [9], [15]. Furthermore, F_3^* is $A(a)$-stable [10] (i.e., fixed-h stable for $\operatorname{Re} q' < -a$) for any $a \geq a_0(q)$. We found that $a_0 = .22435$ for $q = 5$, that $a_0(q)$ is monotone decreasing and, for $q = +\infty$, $a_0 = 1/12 = .08333$ [9]. Finally, for $q = 5$ and $c = 30.708$, F_3^* is $A(r, c)$-stable [10] (i.e., fixed-h stable in $|q' - c| > r$) for any $r \geq r_0 = 31.14$. The center c was chosen in such a way that, approximately, the circle $|q' - c| = r$ is tangent to the image curve of $|w| = 1$ by the map $q'(w) = \rho(w)/\sigma(w)$ at its intersection point with the imaginary axis (so as to reduce to a "minimum" the area cut out of the left half q'-plane by the circle). Again, as q increases from $q = 5$ the $A(r, c)$-stability constraint becomes weaker. For example, the BDF ($q = +\infty$) is $A(r, c)$-stable with $c = 6$ for any $r \geq r_0 = 6.31$ [10]. In Figure 1, the image curve by $q'(w)$ of $|w| = 1$, is plotted for $q = 5, 6$, and $+\infty$ and the bounds of $A(\alpha)$-, $A(a)$-, and $A(r, c)$-stability are shown for $q = 5$.

For $q = +\infty$, the formulas F_k^* are the BDF and are thus trivially A_∞-stable for all k. Because of the continuous dependence of its coefficients on q, $F_k^*(q)$ for any given k must possess this property for any sufficiently large value of q. Similarly, for $q = 0$, the formulas F_k and F_k^* are Adams formulas which are stable [11] (in the limit $q' \to 0$), and even fixed-h stable for a bounded set of values of q'. F_k and F_k^* must thus be stable for any sufficiently small, nonzero value of q.

Of course, $F_k^*(q)$, which for a large value of q is A_∞-stable, may not simultaneously be stable for that value of q. A well-known example of this are the BDF for $k \geq 7$ [9]. Similarly, the stable "near-Adams" formulas $F_k(q)$ and $F_k^*(q)$ associated with small values of q are not A_∞-stable. This lack of uniformity in the stability properties is, however, not a serious drawback for the following reason: In our

matricial integration scheme, the stiff component solutions (corresponding to large values of $q = hd$) are treated by row-formulas fitted at large values of q. These

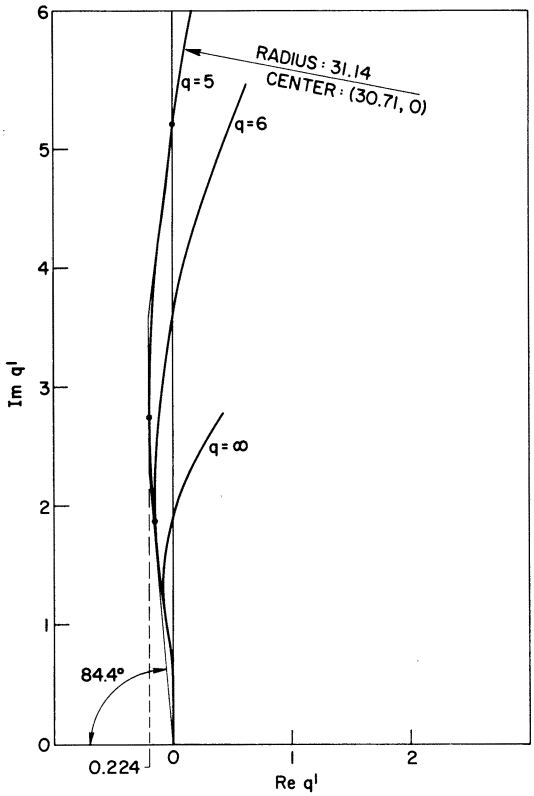

FIGURE 1. *Stability domains for* S3 *as a function of* q.

formulas then possess precisely the unconditional fixed-h stability properties needed to control the stiff components. On the other hand, the slowly varying (smooth, non-stiff) components corresponding to small values of q are treated by Adams-like formulas fitted at those small values of q. These latter formulas then possess precisely the stability—and limited fixed-h stability—properties which are relevant for the smooth components.

As an exception to the lack of uniformity mentioned in the last paragraph, note that F_3^* is stable for all q, $0 \leqslant q \leqslant +\infty$. To show this let $\rho(w, q)$ be the cubic polynomial associated with the α-coefficients of F_3^* and let *** $\hat{\rho}(w, q) = \rho(w, q)/(w - 1)$, a quadratic polynomial. Furthermore, let

$$\hat{r}(z, q) = (z - 1)^2\hat{\rho}((z + 1)/(z - 1)) = 2c_0(q) + 3qc_1(q)z + 3q^2c_2(q)z^2.$$

*** By consistency, $\rho(w, q)$ possesses the linear factor $(w-1)$ for all q.

With appropriate normalization, $c_0(q) = (6 - 9q + 5q^2) + (-6 + 3q + q^2)e^{-q}$, $c_1(q) = (-2 + 3q) + (2 - q)e^{-q}$, and $c_2(q) = 1 - e^{-q}$. Now apply the Routh criterion to $\hat{r}(z, q)$: First $c_2(q) > 0$ for $q > 0$. Next, for $0 < q \leqslant 3$, $c_1'(q) \geqslant q > 0$, $c_1(0) = 0$, and thus $c_1(q) > 0$ for $0 < q \leqslant 3$. For $q \geqslant 3$, $c_1(q) \geqslant 2q > 0$; thus $c_1(q) > 0$ for all q, $0 < q \leqslant +\infty$. Finally, for $q \geqslant q_1 = (-3 + \sqrt{33})/2$, we have $-6 + 3q + q^2 \geqslant 0$ and $c_0(q) \geqslant 6 - 9q + 5q^2 > 0$. For $0 < q \leqslant q_1$,

$$c_0(q) \geqslant (6 - 9q + 5q^2) + (-6 + 3q + q^2)\,[1 - q + (q^2/2)] = (q^3 + q^4)/2 > 0$$

which completes the proof.

4. Algorithmic Implementation.

A. *Newton-Raphson Algorithm.* Algorithms useful for solving stiff systems are generated by applying the Newton-Raphson (NR) method to the nonlinear difference equations associated with the formulas $\mathbf{F}_k^*$ [12]. The derivation is along the lines of [24] and is given in detail in [16]. We give the result of this procedure for $k = 3$. In this case, if a starting guess for the NR method is obtained by quadratic extrapolation from preceding solution values, the NR iteration may be stopped after one step [13].

Let

$$S_0^* = B_{3,0}^*, \qquad S_1^* = -(B_{3,1}^* + B_{3,2}^* + B_{3,3}^*),$$
$$S_2^* = B_{3,2}^* + 2B_{3,3}^*, \qquad S_3^* = -B_{3,3}^*,$$

where the $B_{3,i}^*$, $i = 0, \cdots, 3$, are $(6Q)^{-1}$ times the matrix equivalent of the coefficients β_{3-i} of (3.3), respectively. For the autonomous case of (1.2), the one-step NR algorithm for F_3^* is then defined by the following relations. Let

$$\Delta\tilde{y} = \nabla y + \nabla^2 y, \qquad \tilde{y}^+ = y + \Delta\tilde{y}, \qquad \tilde{\phi}^+ = \phi(\tilde{y}^+),$$
$$\tilde{\phi}_y^+ = \phi_y(\tilde{y}^+), \qquad \phi_y = \partial\phi/\partial y;$$

compute δy^+ by solving

$$(I - hS_0^*\tilde{\phi}_y^+)\delta y^+ = -\Delta\tilde{y} - (I - e^{-Q})y + h(S_0^*\tilde{\phi}^+ - S_1^*\phi - S_2^*\nabla\phi - S_3^*\nabla^2\phi);$$

correct by

$$y^+ = \tilde{y}^+ + \delta y^+, \qquad \nabla^2 y^+ = \nabla^2 y + \delta y^+, \qquad \nabla y^+ = \nabla y + \nabla^2 y^+;$$

and reevaluate:

$$\phi^+ = \phi(y^+), \qquad \nabla\phi^+ = \phi^+ - \phi, \qquad \nabla^2\phi^+ = \nabla\phi^+ - \nabla\phi.$$

As a starting procedure in conjunction with this algorithm, one may use implicit Runge-Kutta methods (see e.g., [25]).

B. *Analysis of the Local Truncation Error.* The error analysis given hereafter is similar to that of [17]. However, we recall that our aim is to derive formulas which are accurate for sufficiently small values of $h\phi$ or of a derivative thereof but for arbitrarily large values of $Q = hD$. Therefore, in analyzing the local truncation error, it is unreasonable to make a complete expansion of this error in powers of h (including

the coefficients of the formula via their dependence on Q). Instead we shall adopt the point of view that Q is an arbitrarily large parameter which we keep constant independently of h. We can, of course, think of this situation as describing a sequence of problems in which we simultaneously vary h and D in an appropriate way.

The formulas we derive hereafter are applicable to the smooth solutions encountered during the asymptotic phase but do not apply to the rapid transients.† In fact, for constant $q > 0$ and $h \to 0$, we have $d \to +\infty$ and in this limit the transient solutions are not smooth. This is exemplified by the case where $\phi(x, y) \equiv 0$, $y' = -dy$, and the solution $y(x) = y_0 e^{-dx}$ for $d = +\infty$ is a step function.

Consider the linear differential difference operator (with $k = p + 1$ for given p)

$$\mathbf{L}_{p+1} = \sum_{j=-p}^{1} \alpha_{j+p}(Q)E^j - h \sum_{j=-p}^{0} \beta_{j+p}(Q)E^j \frac{d}{dx}$$

associated with $\mathbf{F}_{p+1}$, where E is the shift operator. The order of $\mathbf{L}_{p+2}$ exceeds that of $\mathbf{L}_{p+1}$ by one. Therefore, the principal part of the local truncation error of $\mathbf{L}_{p+1}$ is the same as that of $\mathbf{L}_{p+1} - \mathbf{L}_{p+2}$. We find that

$$(\mathbf{L}_{p+1} - \mathbf{L}_{p+2})y(x) = hG_{p+1}\nabla^{p+1}[y'(x) + Dy(x)],$$

where we have substituted $y' + Dy$ for ϕ. For a smooth solution $y(x)$ of (1.2), this yields

$$\begin{aligned}(\mathbf{L}_{p+1} - \mathbf{L}_{p+2})y(x) &= QG_{p+1}\nabla^{p+1}y(x) + hG_{p+1}\nabla^{p+1}y'(x) \\ &= h^{p+1}QG_{p+1}y^{(p+1)}(x) + O(h^{p+2}),\end{aligned}$$

and, from what we have said, it follows that

$$\mathbf{L}_{p+1}y(x) = h^{p+1}QG_{p+1}y^{(p+1)}(x) + O(h^{p+2}). \tag{4.1}$$

Therefore, $\mathbf{F}_{p+1}$ has order of accuracy p when $Q \neq 0$, and $p + 1$ when $Q = 0$; as mentioned before, the latter represents the well-known result for open Adams formulas. In the general case, the coefficient of the principal error term of $\mathbf{L}_{p+1}$ is $C_{p+1} = QG_{p+1}$ according to (4.1).

The error analysis for $\mathbf{F}_p^*$ is analogous to that of $\mathbf{F}_{p+1}$. If (with $k = p$ for given p)

$$\mathbf{L}_p^* = \sum_{j=-(p-1)}^{1} \alpha_{j+p-1}^*(Q)E^j - h \sum_{j=-(p-1)}^{1} \beta_{j+p-1}^*(Q)E^j \frac{d}{dx}$$

is the operator associated with $\mathbf{F}_p^*$, we find that

$$\mathbf{L}_p^* y(x) = h^{p+1}QG_{p+1}^* y^{(p+1)}(x) + O(h^{p+2}).$$

Thus, for $Q \neq 0$, $\mathbf{F}_p^*$ has order of accuracy p. For $Q = 0$ we recover the well-known result that the p-step closed Adams formula, with which $\mathbf{F}_p^*$ is identical in

† This remark relates to the footnote of Section 1.

this case, is of order $p+1$. The coefficient of the principal error term of $\mathbf{L}_p^*$ is $C_{p+1}^* = QG_{p+1}^*$.

We can now write down approximate expressions for the local truncation errors of $\mathbf{F}_{p+1}$ and $\mathbf{F}_p^*$ by the method of Milne [26]. We define a predicted value $\bar{y}_{n+1}^0$ by letting $\mathbf{L}_{p+1}\bar{y}_n^0 = 0$ where, at $x_{n-p}, x_{n-p+1}, \cdots, x_n$, $\mathbf{L}_{p+1}$ operates on the exact solution $y(x)$. One finds that

$$\alpha_{p+1}[\bar{y}_{n+1}^0 - y(x_{n+1})] \simeq -h^{p+1}C_{p+1}y^{(p+1)}(x_n), \tag{4.2}$$

where $\simeq$ denotes equality up to and including $O(h^{p+1})$. Similarly, we define a corrected value y_{n+1}^1 by $\mathbf{L}_p^* y_n^1 = 0$, where for y'_{n+1} we substitute $\bar{\phi}_{n+1}^0 - D\bar{y}_{n+1}^0$, with $\bar{\phi}_{n+1}^0 = \phi(x_{n+1}, \bar{y}_{n+1}^0)$. Then

$$\alpha_p^*[y_{n+1}^1 - y(x_{n+1})] \simeq -h^{p+1}C_{p+1}^* y^{(p+1)}(x_n). \tag{4.3}$$

We can eliminate $y(x_{n+1})$ between (4.2) and (4.3) and solve for $y^{(p+1)}(x_n)$:

$$y^{(p+1)}(x_n) = h^{-(p+1)}[\alpha_{p+1}^{-1}C_{p+1} - \alpha_p^{*-1}C_{p+1}^*]^{-1}(y_{n+1}^1 - \bar{y}_{n+1}^0) + O(h). \tag{4.4}$$

Obviously, α_{p+1} is the identity matrix, whereas

$$\alpha_p^* = I - QB_{p,0}^*.$$

From (4.2) and (4.4), we deduce an estimate for the local truncation error of $\mathbf{F}_{p+1}$,

$$\bar{y}_{n+1}^0 - y(x_{n+1}) \approx \alpha_p^*\hat{G}_{p+1}[\hat{G}_{p+1}^* - \alpha_p^*\hat{G}_{p+1}]^{-1}(y_{n+1}^1 - \bar{y}_{n+1}^0) \tag{4.5}$$

where we have substituted $\hat{G}_{p+1} = (I+Q)G_{p+1}$ for G_{p+1} and $\hat{G}_{p+1}^* = (I+Q)G_{p+1}^*$ for G_{p+1}^*. An expression equivalent to (4.5) would be obtained if we were to replace $\hat{G}$ by G and $\hat{G}^*$ by G^*. But, as $q \to +\infty$, the quantities $\hat{G}(q) \sim qG(q)$ and $\hat{G}^*(q) \sim qG^*(q)$ tend to finite, nonzero limits as we have seen in Section 2. On the other hand $\hat{G} \sim G$ and $\hat{G}^* \sim G^*$ for $q \to 0$, and, in this limit, these quantities in turn have reasonable limits. Thus, relation (4.5) is in a convenient form for computational purposes.

In a very similar manner as for the formula $\mathbf{F}_{p+1}$ we obtain an estimate for the local truncation error of $\mathbf{F}_p^*$:

$$y_{n+1}^1 - y(x_{n+1}) \approx \hat{G}_{p+1}^*[\hat{G}_{p+1}^* - \alpha_p^*\hat{G}_{p+1}]^{-1}(y_{n+1}^1 - \bar{y}_{n+1}^0). \tag{4.6}$$

The error estimates (4.5) and (4.6) can be used for step size control or, as in the next subsection, for defining modifier formulas associated with the predictor and corrector formulas considered above.

C. *Predictor-Corrector Algorithms.* The relations (4.5) and (4.6) can be used to define modified predicted and corrected values. This is done by letting these modified values play the role of $y(x_{n+1})$ in (4.5) and (4.6), by replacing the $\approx$ sign of these relations by the strict equality sign and, in the modifier of the predictor, by shifting the abscissa of $(\bar{y}^0 - y^1)$ back by h. In this sense we arrive at the following one-step predictor-modifier-corrector-modifier (PMCM) algorithm:

$$\bar{y}^0_{n+1} = e^{-Q} y_n + h \sum_{i=-(p-1)}^{1} B_{p,i+p-1}\, \phi_{n-(p-1)-i}, \tag{4.7}$$

$$\bar{y}_{n+1} = \bar{y}^0_{n+1} + \alpha^*_p \hat{G}_{p+1} [\hat{G}^*_{p+1} - \alpha^*_p \hat{G}_{p+1}]^{-1} (\bar{y}^0_{n+1} - y^1_{n+1}), \tag{4.8}$$

$$y^1_{n+1} = e^{-Q} y_n + h \left[B^*_{p,0} \bar{\phi}_{n+1} + \sum_{i=-(p-2)}^{1} B^*_{p,p-1+i} \phi_{n+1-i} \right], \tag{4.9}$$

$$y_{n+1} = y^1_{n+1} + \hat{G}^*_{p+1} [\hat{G}^*_{p+1} - \alpha^*_p \hat{G}_{p+1}]^{-1} (\bar{y}^0_{n+1} - y^1_{n+1}), \tag{4.10}$$

where $\bar{\phi} = \phi(x, \bar{y})$, $\hat{G}_{p+1} = (I + Q) G_{p+1}$, and $\hat{G}^*_{p+1} = (I + Q) G^*_{p+1}$. In the limit $Q \to 0$, the component relations of (4.7) through (4.10) become identical with Adams PMCM algorithms (see e.g., [27] for the cases $p = 2, 3$).

In lieu of the PMCM procedure, it may be advantageous in some cases to use an algorithm in which the formulas (4.7) and (4.8) are combined with a number of applications of the corrector formula,

$$y^i_{n+1} = e^{-Q} y_n + h \left[B^*_{p,0} \phi^{i-1}_{n+1} + \sum_{j=-(p-2)}^{1} B^*_{p,p-1-j} \phi_{n+1-j} \right], \tag{4.11}$$

$$i = 1, 2, \cdots,$$

where $\phi^i = \phi(x, y^i)$ and $\phi^0 = \phi$. The iteration may be stopped when an appropriate measure for the difference between two consecutive corrected values of y becomes smaller than a prescribed threshold. We refer to this as the predictor-modifier-iterated-corrector (PMIC) procedure.

D. *Remark.* If one tries to compute the quantities G_i and G_i^* by the closed expressions of Section 2 the results, because of numerical cancellation, are strongly affected by rounding errors in the limit where a component q of Q satisfies $|q| \ll 1$. It is preferable in this case to compute such components of G_i or G_i^* by power series expansions [16]. It was found by numerical experimentation on an APL system using 56-bit hexadecimal arithmetic, that in computing the quantities g^*_i, $0 \leqslant i \leqslant 3$, a natural separation value q_s, between the range $0 \leqslant q \leqslant q_s$ in which the series evaluation should be used and the range $q_s \leqslant q$ in which the closed expressions seem more accurate, is $q_s = 0.0085$.

5. Numerical Results. The Newton-Raphson algorithm associated with $\mathbf{F}^*_3$—referred to as S3 in the following—was applied to two stiff test problems. The first of these is (a slightly rescaled version of) the first example listed in the survey paper of Bjurel et al. [28, Section 4, p. 1], and is due to Fowler and Warten [29]. This problem, which will be referred to as P1, is defined by the equations and initial conditions

$$\text{P1} \begin{cases} y_1' = -2000 y_1 + 1000 y_2 + 1000, & y_1(0) = 0, \\ y_2' = y_1 - y_2, & y_2(0) = 0. \end{cases}$$

Its exact solution is given in [16]. Near $x = 0$ the solution to P1 has a "boundary

layer" in the y_1-component, of amplitude ≈ 0.5. To avoid this area, the numerical integration was actually carried out in the interval $1 \leqslant x \leqslant 4$, using the exact solution values at $x_0 = 1, x_1 = 1 + h,$ and $x_2 = 1 + 2h$ as starting values. The relative accumulated truncation error in absolute value was computed and maximized over the abscissa values $x_i = 1 + i \times 0.6,\ i = 0, \cdots, 5$. The second component (the larger one) of this error is plotted in Figure 2 as a function of h. The curve labelled S3 represents the results by the third order algorithm S3 using $d_1 = 2000$ and $d_2 = 1$. For comparison, the results of the third order algorithm A3 of [24] is plotted under this label, and the results obtained by the BDF with $k = p = 3$, implemented as S3 with $d_1 = d_2 = 10^5$ (in place of $+\infty$), is plotted as curve BDF3. We find that, for this linear problem with constant coefficients, the algorithm S3 is considerably more accurate than either BDF3 or A3, despite the fact that the off-diagonal terms are not small compared to the diagonal ones. It should be remembered, however, that A3 was designed to be A-stable whereas S3 is not A-stable. The order of accuracy reflects itself in the slope of the approximately straight-line curves. The theory predicts that the accumulated truncation error is $O(h^p)$, $p = 3$. In accordance with this the three curves have a slope of $-p \approx -3$ in this manner of plotting.

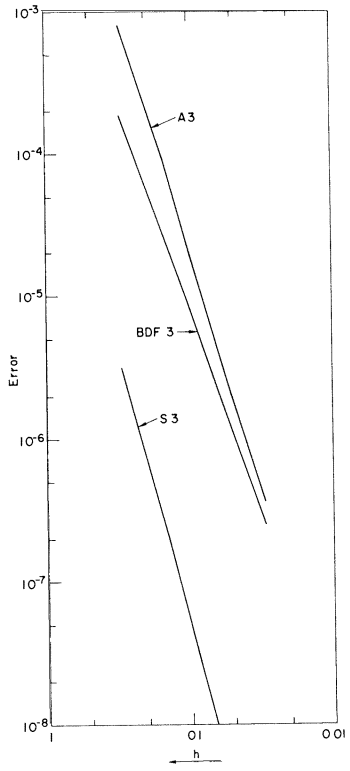

FIGURE 2. *Accumulated truncation errors for test problem* P1.

As a second test problem we solved the nonlinear system [24]

$$\text{P2} \begin{cases} y_1' = 0.01 - [1 + (1000 + y_1)(1 + y_1)](0.01 + y_1 + y_2), \\ y_2' = 0.01 - (1 + y^2)(0.01 + y_1 + y_2), \end{cases}$$

from $x = 1$ through $x = 81$. As starting values near $x = 1$ we used values of the "exact" solution defined by $y_1(0) = y_2(0) = 0$ and computed by the well-known fourth-order Runge-Kutta method with an extremely small step, $h = .002$. The eigenvalues are $\lambda_1 \approx -981$, $\lambda_2 \approx -2 \times 10^{-5}$ at $x = 1$, and $\lambda_1 \approx -185$, $\lambda_2 \approx -10^{-3}$ at $x = 81$. The numerical results of applying the algorithms S3 with $d_1 = 1011.01$ and $d_2 = 1$, A3, and BDF3 to P2 are plotted in Figure 3 in a similar manner as for P1 in Figure 2. Again the algorithm S3 proves to be more accurate than A3 and BDF3, although the difference in this nonlinear problem is not as great as in P1.

For both problems, calculations have been carried out with values of D other than the two associated with the curves labelled A3 and BDF, respectively. The

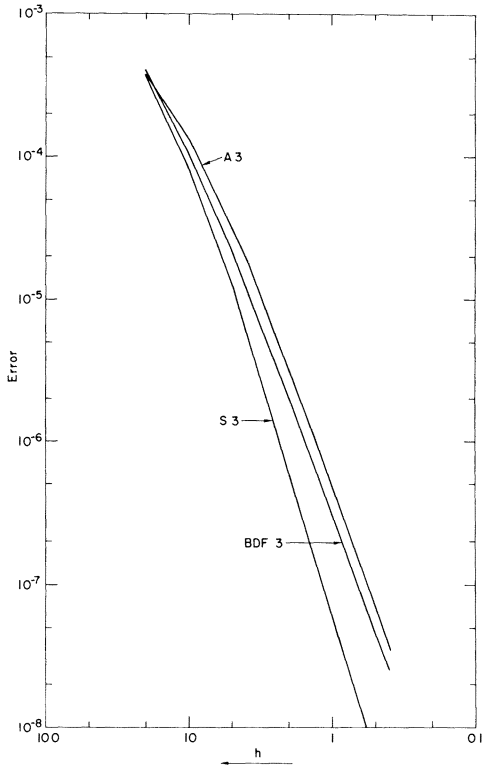

FIGURE 3. *Accumulated truncation errors for test problem* P2.

esults generally showed a low sensitivity to reasonable changes of D within the stability constraints given in Section 3.

The third-order PMCM and PMIC procedures were tested on five stiff or diagonally dominant, nonstiff problems [16]. In summary, the following observations were made in these tests: As far as stiff problems are concerned, the PMIC procedure yielded useful, though somewhat erratic results even with relatively large integration steps. Instead, as expected, open methods such as PMCM, Adams, and explicit Runge-Kutta procedures broke down for all but the smallest step sizes used. With small integration steps, PMCM appeared to be more accurate than the corresponding third-order Adams procedure (which is the special case of PMCM fitted at $Q = 0$), or the standard fourth-order Runge-Kutta method. Similarly, for nonstiff problems and for intermediate step sizes at which Adams and Runge-Kutta are still stable, the exponentially fitted algorithms PMCM and PMIC proved to be more accurate than the former methods. As one might expect, the gain was greater in linear than in nonlinear problems.

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