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ON EXTRAPOLATION ALGORITHMS FOR ORDINARY INITIAL VALUE PROBLEMS*

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1. Introduction. The algorithm of Romberg [20], [3] and its generalizations [4], [5] for the numerical evaluation of definite integrals are based on the fact that, under suitable regularity assumptions on the integrand, the trapezoidal approximation with step h has an asymptotic expansion in powers of h^2. It is proposed in [3], [5] to apply similar ideas to the solution of first order ordinary initial value problems using Euler's method as the basic discretization. The corresponding asymptotic expansion then contains also odd powers of h. The main purpose of this paper is to establish the existence of simple discretizations of both first and special second order systems which have asymptotic expansions in powers of h^2. These schemes, coupled with a slower mesh refinement [4] and the use of rational function extrapolation [5] should lead to effective algorithms of this type for ordinary initial value problems. Numerical results are given for the restricted two body problem, including comparison with some classical techniques.

2. Extrapolation schemes. Let $D(h)$ be a complex valued discrete approximation defined for *steps* $h \in H = (0, h_0]$ to the solution $D(0)$ of an infinitesimal problem. Under the assumption that $D(h)$ has an *asymptotic expansion*

$$D(h) \sim e_0 + e_1 h^2 + e_2 h^4 + \cdots, \qquad h \in H, \tag{2.1}$$

Richardson [18], [19] proposed to obtain improved approximations from two or more values of $D(h)$, say at $h_0 > h_1 > \cdots > h_n$, by requiring that the linear combinations

$$p_0^{(n)} \equiv \sum_{m=0}^{n} c_m^{(n)} D(h_m)$$

satisfy

$$p_0^{(n)} = D(0) + O(h_0^{2n+2}), \qquad h_0 \to 0^+.$$

It is important that the constants $c_m^{(n)}$ need not be calculated. The $p_0^{(n)}$ can be found indirectly with the Neville algorithm for the recursive construction of $p_n^{(m)} \equiv p_n^{(m)}(0)$, where $p_n^{(m)}(h^2)$ is the polynomial of degree m in h^2 which interpolates $D(h)$ at $h = h_k$, $k = n, \cdots, n + m$. One

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forms the triangular array

$$\begin{array}{cccccc}
p_0^{(0)} & & & & & \\
& p_0^{(1)} & & & & \\
p_1^{(0)} & & p_0^{(2)} & & & \\
& p_1^{(1)} & & p_0^{(3)} & & \\
& & \searrow & \cdot & \cdot & \\
p_2^{(0)} & & p_1^{(2)} & \cdot & & \cdot \\
& & \nearrow \cdot & \cdot & & \cdot \\
& p_2^{(1)} & \cdot & & & \\
& \cdot & \cdot & & & \\
p_3^{(0)} & \cdot & & & & \\
\cdot & \cdot & & & & \\
\cdot & & & & & \\
\cdot & & & & &
\end{array}$$

from the linear recursion

$$\begin{aligned} p_n^{(0)} &= D(h_n), \\ p_n^{(m)} &= p_{n+1}^{(m-1)} + \frac{p_{n+1}^{(m-1)} - p_n^{(m-1)}}{(h_n/h_{n+m})^2 - 1}. \end{aligned} \tag{2.2}$$

For the applications discussed in this paper the main computational effort occurs in the evaluation of the first column. The scheme is built up by generating, at the nth stage, the upward sloping diagonal beginning with $p_n^{(0)}$. See, for example, the algorithms in [2], [5].

The following theorem states that, under mild assumptions on $D(h)$ and the rate of refinement of the mesh, the linear sequence to sequence transformation $p_n^{(0)} \to p_0^{(n)}$ of the first column into the diagonal is convergence and limit preserving. The sufficiency was stated, in a special case, by Stiefel and Rutishauser [23]. A more general theorem is that of Laurent [14].

THEOREM 2.1. *A necessary and sufficient condition that* $\lim_{n\to\infty} p_0^{(n)} = D(0)$ *for all functions* $D(h)$ *continuous from the right at* $h = 0$ *is that*

$$\alpha = \sup_{n\geqq 0} \frac{h_{n+1}}{h_n} < 1. \tag{2.3}$$

In particular, (2.3) implies the Toeplitz condition

$$C = \sup_{n\geqq 0} \sum_{m=0}^{n} | c_m^{(n)} | < \infty. \tag{2.4}$$

The constant C is a measure of the numerical stability of the scheme. The sequences $h(\alpha)$, $0 < \alpha \leqq 1$, defined by

$$h_n(\alpha) = \frac{h_0}{k_n}, \qquad \begin{cases} k_0 = 1, \\ k_{n+1} = \text{entier}\,(k_n/\alpha) + 1, \end{cases} \tag{2.5}$$

give the following values for $C(\alpha)$:

(2.6)

α	$\frac{1}{2}^{+}$	$\frac{4}{7}$	$\frac{2}{3}$	$\frac{8}{11}$	$\frac{4}{5}$	$\frac{8}{9}$	1
$C(\alpha)$	1.97	2.71	5.4	11	48	4850	$+\infty$

The next theorem provides statements about the rates of convergence of the columns and principal diagonal of the p-scheme. It follows from results in [11], [5].

THEOREM 2.2. *Let* $D(h)$ *have the asymptotic expansion* (2.1) *and let* $\sup_{n\geqq 0} h_{n+1}/h_n \leqq \alpha < 1$. *Then, as* $n \to \infty$,

$$p_n^{(m)} - D(0) = (-1)^m e_{m+1}(h_n \cdots h_{n+m})^2 + o((h_n \cdots h_{n+m})^2). \tag{2.7}$$

If, in addition, $0 < \beta \leqq \inf_{n\geqq 0} h_{n+1}/h_n$ *then there exist constants* E_m *such that, for each* $m \geqq 0$,

$$|p_0^{(n)} - D(0)| \leqq E_{m+1}(h_n \cdots h_{n+m})^2, \qquad n \geqq 0. \tag{2.8}$$

In the normal case where $e_m \neq 0$, $m = 1, 2, \cdots$, (2.7) states that each column of the p-scheme converges to $D(0)$ faster than the preceding one, and (2.8) shows that the principal diagonal converges faster than any column. Under mild restrictions on the rate of growth of the order constants implied by (2.1), it can be shown that $p_0^{(n)}$ converges *superlinearly* to $D(0)$ in the sense that $|p_0^{(n)} - D(0)| \leqq K_n$ and $\lim_{n\to\infty} K_{n+1}/K_n = 0$. Such is the case if $D(h)$ can be extended to a function which is analytic at $h = 0$.

An important generalization of (2.2) has recently been proposed in [5]. It uses the algorithm of Stoer [24] to construct $r_n^{(m)} = r_n^{(\mu,\nu)}(0)$, where $r_n^{(\mu,\nu)}(h^2)$ is "the" rational function with numerator degree μ and denominator degree ν $(\mu + \nu = m)$ which interpolates $D(h)$ at $h = h_k$, $k = n$, $\cdots$, $n + m$. Choosing the sequence $(\mu, \nu) = (0, 0), (0, 1), (1, 1), (1, 2)$, $\cdots$ gives the nonlinear recursion

$$r_n^{(-1)} = 0, \qquad r_n^{(0)} = D(h_n),$$

$$r_n^{(m)} = r_{n+1}^{(m-1)} + \frac{r_{n+1}^{(m-1)} - r_n^{(m-1)}}{\left(\dfrac{h_n}{h_{n+m}}\right)^2 \left[1 - \dfrac{r_{n+1}^{(m-1)} - r_n^{(m-1)}}{r_{n+1}^{(m-1)} - r_{n+1}^{(m-2)}}\right] - 1} \tag{2.9}$$

with the diagram

$$\begin{tikzcd}
r_n^{(m-2)} & & \\
& r_n^{(m-1)} \arrow[dr] & \\
r_{n+1}^{(m-2)} \arrow[rr] & & r_n^{(m)} \\
& r_{n+1}^{(m-1)} \arrow[ur] & \\
r_{n+2}^{(m-2)} & &
\end{tikzcd}$$

A statement analogous to that of Theorem 2.2 on the rate of convergence of the columns of the Stoer scheme involves the Hankel determinants

$$H_p^{(q)} = \begin{vmatrix} e_p & e_{p+1} & \cdots & e_{p+q-1} \\ e_{p+1} & e_{p+2} & \cdots & e_{p+q} \\ \vdots & \vdots & & \vdots \\ e_{p+q-1} & e_{p+q} & \cdots & e_{p+2q-2} \end{vmatrix}.$$

THEOREM 2.3. *In addition to the hypotheses of Theorem 2.2 let* $H_p^{(q)} \neq 0$, $p = 0, 1, q = 1, 2, \cdots$. *If* h_0 *is sufficiently small the* mth *column of the Stoer scheme exists and*

$$r_n^{(m)} - D(0) \sim (-1)^m \tilde{e}_{m+1}(h_n \cdots h_{n+m})^2, \qquad n \to \infty,$$

where

$$\tilde{e}_{2q} = \frac{H_0^{(q+1)}}{H_0^{(q)}}, \qquad \tilde{e}_{2q+1} = \frac{H_1^{(q+1)}}{H_1^{(q)}}.$$

The algorithm of Romberg [20] for the evaluation of definite integrals,

$$T(0) = \int_a^b f(t)\,dt, \qquad \begin{cases} I = [a, b] \text{ finite}, \\ f \in C^\infty(I), \end{cases}$$

has been studied in the interesting papers [1], [23], [22], [3] by Bauer, Rutishauser, and Stiefel and, for more general h-sequences, by Bulirsch [4]. The discretization is the *trapezoidal rule*

$$(2.10) \quad T(h) = h[\tfrac{1}{2}f(a) + f(a+h) + \cdots + f(b-h) + \tfrac{1}{2}f(b)]$$

which, according to the Euler-Maclaurin formula, has the asymptotic expansion

$$(2.11) \qquad T(h) \sim T(0) + \sum_{m=1}^{\infty} \frac{B_{2m}}{(2m)!}[f^{(2m-1)}(b) - f^{(2m-1)}(a)]h^{2m}.$$

The B_{2m} are the Bernoulli numbers

$$\frac{B_{2m}}{(2m)!} = \frac{2(-1)^{m-1}\zeta(2m)}{(2\pi)^{2m}},$$

and $\zeta(z)$ is the Riemann zeta function. If f is analytic on I then (2.3) implies that $p_0^{(n)} \to T(0)$ superlinearly as $n \to \infty$.

One can also base similar schemes on the *midpoint rule*

$$M(h) = h\left[f\left(a + \frac{h}{2}\right) + f\left(a + \frac{3h}{2}\right) + \cdots + f\left(b - \frac{h}{2}\right)\right].$$

Since

$$(2.12) \qquad T\left(\frac{h}{2}\right) = \frac{1}{2}[T(h) + M(h)],$$

the Euler-Maclaurin formula shows that (2.1) holds for $M(h)$ with

$$e_m = -\left(1 - \frac{2}{4^m}\right)\frac{B_{2m}}{(2m)!}[f^{(2m-1)}(b) - f^{(2m-1)}(a)].$$

The relation (2.12) was used by Romberg, with the sequence $h(\frac{1}{2}^+)$, to construct the first column of his T-scheme.

3. Two one-step methods for first order systems. Let f be continuous and uniformly Lipschitzian with respect to its second argument on the set $D = I \times C_l$, where $I = [a, b]$ is a finite t-interval and C_l is the complex normed linear space of l-tuples $x = (x^{(1)}, \cdots, x^{(l)})$. Let it be required to find $\phi(t)$ at a fixed point $t = a + h_0 \in I$, where ϕ is the unique solution of the initial value problem

$$\begin{aligned} x(a) &= s, \\ x' &= f(t, x), \qquad t \in I. \end{aligned} \tag{3.1}$$

If $\phi(t)$ is wanted at a number of points $t \in I$ the algorithms described below, coupled with the extrapolation schemes (2.2) or (2.9), can be applied over the subintervals between successive points. When $l > 1$ the extrapolation schemes are applied to the individual components of the numerical solution. Two familiar one-step methods are considered in this section: Euler's method and the usual generalization to differential equations of the trapezoidal rule. For the special case where f is independent of x, their asymptotic expansions reduce to the Euler-Maclaurin formula (2.11). The proofs, which are easier than the proof of Theorem 4.2, appear in [11], [21].

It is assumed further that $f \in C^\infty(D)$. Denote by J the Jacobian matrix of f, evaluated at the solution ϕ,

$$J(t) = \frac{\partial f}{\partial x}(t, \phi(t)), \quad t \in I,$$

and define the symmetric k-linear operators $f^{(k)}(t, \phi(t))$, $t \in I$, from C_l to C_l by

$$f^{(k)}(t, \phi(t))x_1 \cdots x_k = \sum_{l_1=1}^{l} \cdots \sum_{l_k=1}^{l} \frac{\partial^k f(t, \phi(t))}{\partial x_1^{(l_1)} \cdots \partial x_k^{(l_k)}} x_1^{(l_1)} \cdots x_k^{(l_k)}.$$

The properties of such operators are discussed in [15]. This device reduces the formal study of systems to that of a single differential equation.

The coefficients of several asymptotic expansions to be given below can be defined as solutions of certain recursive systems of linear differential equations. Put

(3.2a) $$e_0(t) \equiv \phi(t),$$

and, for $m = 1, 2, \cdots$, let $e_m(t)$ satisfy

(3.2b) $$\begin{aligned} e_m(a) &= 0, \\ e_m' &= J(t)e_m + a_m(t) + b_m(t), \qquad t \in I, \end{aligned}$$

where

(3.2c) $$a_m(t) = -\sum_{k=1}^{m} \alpha_k e_{m-k}^{(qk+1)}(t)$$

and

(3.2d) $$\sum_{m=1}^{\infty} b_m(t)z^m \equiv \sum_{k=2}^{\infty} \frac{1}{k!} f^{(k)}(t, \phi(t)) \left(\sum_{m=1}^{\infty} e_m(t)z^m \right)^k.$$

The integer q and constants α_k will be specified in each particular case by the generating function

(3.2e) $$A(z) = \sum_{k=0}^{\infty} \alpha_k z^{qk}.$$

It was proposed in [3], [5] to use Euler's method as a simple discretization of (3.1). Thus put

$$E(t; h) = x_N(h), \qquad Nh = t - a,$$

where the sequence $x_n(h)$, $n = 0, \cdots, N$, satisfies the difference equation

$$x_0 = s,$$

$$x_{n+1} = x_n + hf(t_n, x_n),$$

with $t_n = a + nh$.

THEOREM 3.1. *Let the functions $e_m(t)$ be defined by* (3.2) *with*

$$A(z) = \frac{e^z - 1}{z} = \sum_{k=0}^{\infty} \frac{1}{(k+1)!} z^k.$$

Then

(3.3) $$E(t; h) \sim e_0(t) + e_1(t)h + e_2(t)h^2 + \cdots$$

uniformly for $t \in I$ and steps $h \in H$.

Since (3.3) contains odd powers of h the extrapolation schemes must be modified in an obvious way. For example, the Neville scheme becomes

$$p_n^{(m)} = p_{n+1}^{(m-1)} + \frac{p_{n+1}^{(m-1)} - p_n^{(m-1)}}{\dfrac{h_n}{h_{n+m}} - 1}.$$

This results in a loss of numerical stability. Some values of the corresponding constants $C(\alpha)$ (see (2.4)–(2.6)) are:

α	$\frac{1}{2}^+$	$\frac{4}{7}$	$\frac{2}{3}$	$\frac{8}{11}$	$\frac{4}{5}$	$\frac{8}{9}$	1
$C(\alpha)$	8.3	17.4	79	370	8500	$>10^8$	$+\infty$

Note that, for the differential equation $x(0) = s$, $x' = ax$, $a =$ const.,

$$E(t; h) = (1 + ah)^N s = \exp\left[at \frac{\log(1 + ah)}{ah}\right] s$$
$$= e^{at}[1 + p_1(at)ah + p_2(at)(ah)^2 + \cdots]s$$

is analytic for $|h| < 1/|a|$. The $p_m(t)$ are polynomials of degree m. It follows from this and a previous remark that if $\alpha < 1$ then $p_0^{(n)} \to e^{at}s$ superlinearly for the Neville scheme. However, this superlinear convergence is slower for larger values of $|a|$. This behavior generalizes to the other methods studied below.

An obvious choice for a discretization of (3.1) with an h^2-expansion is the usual generalization of the trapezoidal rule:

$$T(t; h) = x_N(h), \qquad Nh = t - a,$$

with

$$x_0 = s,$$

$$x_{n+1} = x_n + \frac{h}{2}[f(t_{n+1}, x_{n+1}) + f(t_n, x_n)]. \tag{3.4}$$

THEOREM 3.2. *Let the functions $e_m(t)$ be defined by* (3.2) *with*

$$A(z) = \frac{2}{z}\tanh\left(\frac{z}{2}\right) = \left(\sum_{k=0}^{\infty} \frac{B_{2k}}{(2k)!} z^{2k}\right)^{-1}.$$

If h_0 is sufficiently small the difference equation (3.4) *has a unique solution $x_n(h)$, $n = 0, \cdots, N$, and*

$$T(t; h) \sim e_0(t) + e_1(t)h^2 + e_2(t)h^4 + \cdots$$

uniformly for $t \in I$ and steps $h \in H$.

This generalization of the trapezoidal rule (2.10) has an important stability property. It has been shown by Dahlquist [7], [8] that any linear multistep method which preserves the asymptotic stability of solutions of $x' = Ax$, Re $\lambda(A) < 0$, for all $h > 0$ necessarily is of order $\leqq 2$ and that, among the second order methods with this property, the trapezoidal rule has the smallest error constant. This is of interest when A has some eigenvalues with large negative real parts so that the general solution contains rapidly decaying transients. The trapezoidal rule prevents these components from reentering the numerical solution once they have decayed. Dahlquist then proposes using *global* extrapolation to increase the order of the approximation.

It is not possible to base a general purpose procedure on extrapolation of the trapezoidal rule since the h^2-expansion does not hold unless the system (3.4) is solved exactly at each step. The classical predictor-corrector technique requires in general infinitely many evaluations of f to obtain the h^2-expansion. On the other hand, if it is relatively easy to solve (3.4) exactly the use of extrapolation gives very good results.

4. A composite rule. The starting point for the main result on first order systems is Nyström's second order method, commonly called the midpoint rule:

$$\begin{aligned} \mathfrak{N}(t; h) &= x_N(h), \qquad Nh = t - a, \\ x_0 &= s, \qquad x_1 = s_1(h), \\ x_{n+1} &= x_{n-1} + 2hf(t_n, x_n). \end{aligned} \tag{4.1}$$

This is a two-step method and thus requires an additional starting value $s_1(h)$. It is the simplest linear k-step method [6],

$$\rho(E)x_n = h\sigma(E)f(t_n, x_n),$$

which is symmetric in the sense that

$$\rho(z) + z^k\rho(z^{-1}) = \sigma(z) - z^k\sigma(z^{-1}) = 0.$$

The requirement of stability implies that all zeros of $\rho(z)$ are of unit modulus for a symmetric method. If $k > 1$ and negative growth parameters exist, weak instability can occur. This is less important in the step-by-step use of symmetric methods with extrapolation schemes. It does require a moderate control of the step h_0, however.

For symmetric methods it is theoretically possible, by a suitable choice of starting values, to obtain asymptotic expansions in powers of h^2. The following theorem was given, in part, by de Vogeleare [9] who extended a result of Gaunt [10]. It generalizes easily to the class of symmetric multistep methods.

THEOREM 4.1. *Let the functions* $e_m(t)$ *be defined by* (3.2) *with*

$$A(z) = \frac{\sinh z}{z} = \sum_{k=0}^{\infty} \frac{1}{(2k+1)!} z^{2k}.$$

If the starting function $s_1(h)$ *satisfies*

$$\begin{aligned} s_1(h) &\sim e_0(a+h) + e_1(a+h)h^2 + e_2(a+h)h^4 + \cdots \\ &\sim \phi(a) + \phi'(a)h + \tfrac{1}{2}\phi''(a)h^2 - \tfrac{1}{12}[J(a)\phi'''(a) + \tfrac{1}{2}\phi^{(4)}(a)]h^4 + \cdots \end{aligned} \tag{4.2}$$

for $h \in H$, *then*

$$\mathfrak{N}(t; h) \sim e_0(t) + e_1(t)h^2 + e_2(t)h^4 + \cdots$$

uniformly for $t \in I$ *and steps* $h \in H$.

Note that (4.2) does not require $s_1(h) \equiv \phi(a + h)$. It is difficult to obtain since it requires a knowledge of J and high order derivatives of the solution ϕ. De Vogeleare proposes the use of methods of Runge-Kutta type to satisfy (4.2) approximately. This appears cumbersome and in general does not lead to an infinite h^2-expansion.

The most natural choice for the starting function $s_1(h)$, in terms of the data of the problem (3.1), is

$$s_1(h) = s + f(a, s)h. \tag{4.3}$$

It is a remarkable fact that this choice leads to a certain type of *infinite* h^2-expansion. The statement of this result requires the recursive definition, similar to (3.2), of *two* sequences of functions $e_m(t), f_m(t)$. Put

$$e_0(t) = f_0(t) \equiv \phi(t), \tag{4.4a}$$

and, for $m = 1, 2, \cdots$, let $e_m(t), f_m(t)$ satisfy

$$\begin{aligned} e_m(a) &= 0, \qquad f_m(a) = -\sum_{k=1}^{m} \frac{1}{(2k)!} f_{m-k}^{(2k)}(a), \\ e_m' &= J(t)f_m + a_m(t) + b_m(t), \qquad f_m' = J(t)e_m + c_m(t) + d_m(t), \\ & \qquad\qquad t \in I, \end{aligned} \tag{4.4b}$$

where

$$\begin{aligned} a_m(t) &= -\sum_{k=1}^{m} \frac{1}{(2k+1)!} e_{m-k}^{(2k+1)}(t), \\ c_m(t) &= -\sum_{k=1}^{m} \frac{1}{(2k+1)!} f_{m-k}^{(2k+1)}(t), \end{aligned} \tag{4.4c}$$

and

$$\begin{aligned} \sum_{m=1}^{\infty} b_m(t)z^m &\equiv \sum_{k=2}^{\infty} \frac{1}{k!} f^{(k)}(t, \phi(t)) \left(\sum_{m=1}^{\infty} f_m(t)z^m\right)^k, \\ \sum_{m=1}^{\infty} d_m(t)z^m &\equiv \sum_{k=2}^{\infty} \frac{1}{k!} f^{(k)}(t, \phi(t)) \left(\sum_{m=1}^{\infty} e_m(t)z^m\right)^k. \end{aligned} \tag{4.4d}$$

THEOREM 4.2. *Let* $\mathfrak{N}(t; h)$ *be constructed from the algorithm* (4.1) *with* $s_1(h) = s + f(a, s)h$. *Then*

$$\mathfrak{N}(t; h) \sim \sum_{m=0}^{\infty} \begin{Bmatrix} e_m(t) \\ f_m(t) \end{Bmatrix} h^{2m}, \qquad t \in I, h \in H. \tag{4.5}$$

The upper (*lower*) *expression is taken when* N *is even* (*odd*).

This result shows that there exist two distinct h^2-expansions arising from Nyström's method with the starting function (4.3). Extrapolation is therefore possible with a sequence of even N's *or* with a sequence of odd N's. Since $e_m(a) = 0$ but in general $f_m(a) \not\equiv 0$ for $m \geqq 1$, the former procedure is perhaps preferred. To better understand Theorem 4.2, put

$$u_m(t) = \tfrac{1}{2}[e_m(t) + f_m(t)], \qquad v_m(t) = \tfrac{1}{2}[e_m(t) - f_m(t)],$$

and compare with Theorem 4.2 of Henrici [13]. The functions u_m and v_m satisfy differential equations of the form

$$u_m' = J(t)u_m + \text{inhomogeneous terms},$$

$$v_m' = -J(t)v_m + \text{inhomogeneous terms};$$

the expansion (4.5) becomes

$$\mathfrak{N}(t; h) \sim \sum_{m=0}^{\infty} [u_m(t) + (-1)^N v_m(t)]h^{2m}. \tag{4.6}$$

The functions v_m are the "weakly unstable" components of the discretization error. Note that $v_0(t) \equiv 0$. By choosing a more *accurate* starting value $s_1(h)$, it is possible to obtain an expansion of the form (4.6) where, in addition, $v_1(t) \equiv 0$. Such is the case if

$$s_1(h) = \phi(a) + \phi'(a)h + \tfrac{1}{2}\phi''(a)h^2,$$

but this requires the knowledge of $f_t(a, s)$ and $J(a)$. Even then $v_2(t) \not\equiv 0$ in general. It will be seen later how to annihilate $v_1(t)$ which is the leading unstable component.

Proof of Theorem 4.2. For $p \geqq 1$ and $t = t_n = a + nh$ let

$$\epsilon_n(h) \equiv x_n(h) - \phi(t) - \delta_n(h),$$

$$\delta_n(h) \equiv \sum_{m=1}^{p-1} \begin{Bmatrix} e_m(t) \\ f_m(t) \end{Bmatrix} h^{2m}, \qquad n \begin{Bmatrix} \text{even} \\ \text{odd} \end{Bmatrix}.$$

It will be shown that $\epsilon_n(h) = O(h^{2p})$ uniformly for $t \in I$ and steps $h \in H$. This is known for $p = 1$ [13, Theorem 4.1]; thus

$$\epsilon_n(h) = O(h^2), \qquad t \in I, h \in H. \tag{4.7}$$

Define the linear operator $\mathfrak{L}$ by

$$\mathfrak{L}\epsilon_n = \epsilon_{n+1} - \epsilon_{n-1} - 2hJ(t)\epsilon_n .$$

For $p > 1$ the result will follow from

$$\epsilon_0(h) = 0, \qquad \epsilon_1(h) = O(h^{2p}), \tag{4.8a}$$

$$\mathfrak{L}\epsilon_n(h) = O(h^3 \| \epsilon_n(h) \|) + O(h^{2p+1}), \qquad t \in I, h \in H, \tag{4.8b}$$

by (4.7) and $p - 1$ applications of [13, Lemma 3.2].

The first equation of (4.8a) holds since $x_0(h) = s = \phi(a)$ and $e_m(a) = 0$, $m = 1, 2, \cdots$. Similarly

$$\epsilon_1(h) = \phi(a) + \phi'(a)h - \sum_{m=0}^{p-1} f_m(a + h)h^{2m}.$$

Expanding $f_m(a + h)$ in finite Taylor series about $h = 0$, rearranging into powers of h, and estimating remainders gives

$$-\epsilon_1(h) = \sum_{m=0}^{p-1} \left[f_m(a) + \sum_{k=1}^{m} \frac{1}{(2k)!} f_{m-k}^{(2k)}(a) \right] h^{2m}$$

$$+ \sum_{m=0}^{p-1} \left[f_m'(a) + \sum_{k=1}^{m} \frac{1}{(2k+1)!} f_{m-k}^{(2k+1)}(a) \right] h^{2m+1} + O(h^{2p}), \qquad h \in H.$$

The sums vanish because of the initial value problems defining the f_m. By (4.4d), $d_m(a) = 0$ since $e_m(a) = 0$. This completes the proof of (4.8a).

To show (4.8b), write

$$\mathcal{L}\epsilon_n = \mathcal{L}x_n - \sum_{m=0}^{p-1} \mathcal{L} \begin{Bmatrix} e_m(t) \\ f_m(t) \end{Bmatrix} h^{2m} \tag{4.9}$$

and consider each term on the right separately. From the difference equation (4.1),

$$\mathcal{L}x_n = 2h[f(t, \phi(t) + \delta_n + \epsilon_n) - J(t)(\phi(t) + \delta_n + \epsilon_n)].$$

Expanding $f(t, \phi(t) + \delta_n + \epsilon_n)$ in a finite (Fréchet) Taylor series about $\phi(t)$ and estimating remainders, using the fact that both $\delta_n(h)$ and $\epsilon_n(h)$ are uniformly $O(h^2)$, gives

$$f(t, \phi(t) + \delta_n + \epsilon_n) - f(t, \phi(t)) - J(t)(\delta_n + \epsilon_n)$$

$$= \sum_{k=2}^{p-1} \frac{1}{k!} f^{(k)}(t, \phi(t))(\delta_n + \epsilon_n)^k + O(h^{2p})$$

$$= \sum_{k=2}^{p-1} \frac{1}{k!} f^{(k)}(t, \phi(t))\delta_n^{\,k} + O(h^2 \| \epsilon_n \|) + O(h^{2p}), \qquad t \in I, h \in H.$$

Combining the last two expressions with (4.4d) yields

$$\begin{aligned} \mathcal{L}x_n = 2h &\left[f(t, \phi(t)) - J(t)\phi(t) + \sum_{m=1}^{p-1} \begin{Bmatrix} d_m(t) \\ b_m(t) \end{Bmatrix} h^{2m} \right] \\ &+ O(h^3 \| \epsilon_n \|) + O(^{2p+1}), \qquad t \in I, h \in H. \end{aligned} \tag{4.10}$$

The mth term of the sum (4.9) can be expanded similarly:

$$\mathfrak{L}\begin{Bmatrix} e_m(t) \\ f_m(t) \end{Bmatrix} = \begin{Bmatrix} f_m(t+h) - f_m(t-h) - 2hJ(t)e_m(t) \\ e_m(t+h) - e_m(t-h) - 2hJ(t)f_m(t) \end{Bmatrix}$$

$$= 2h\left[\begin{Bmatrix} f_m'(t) - J(t)e_m(t) \\ e_m'(t) - J(t)f_m(t) \end{Bmatrix} + \sum_{k=1}^{p-m-1} \frac{1}{(2k+1)!}\begin{Bmatrix} f_m^{(2k+1)}(t) \\ e_m^{(2k+1)}(t) \end{Bmatrix} h^{2k}\right]$$

$$+ O(h^{2(p-m)+1}), \qquad t \in I, h \in H.$$

Rearranging into powers of h^2 and applying (4.4c) then gives

$$\mathfrak{L}\sum_{m=0}^{p-1}\begin{Bmatrix} e_m(t) \\ f_m(t) \end{Bmatrix} h^{2m} = 2h\sum_{m=0}^{p-1}\begin{Bmatrix} f_m'(t) - J(t)e_m(t) - c_m(t) \\ e_m'(t) - J(t)f_m(t) - a_m(t) \end{Bmatrix} h^{2m}$$

$$+ O(h^{2p+1}), \qquad t \in I, h \in H.$$

The verification of (4.8) is completed by combining this with (4.9–10) and recalling the differential equations (3.1), (4.4b).

Because of Theorem 4.2 it seems natural to separate the "even" and "odd" parts of $\mathfrak{N}(t; h)$. Also, noting the special case of ordinary integration when $f(t, x)$ is independent of x, one is led to define generalizations of $M(h)$ and $T(h)$ by

$$M(t; h) = x_N(h), \qquad Nh = t - a,$$

$$T(t; h) = y_N(h) - \frac{h}{2}f(t, x_N(h)),$$

where

$$x_0 = s, \qquad y_0 = s + \frac{h}{2}f(a, s),$$

$$x_{n+1} = x_n + hf(t_{n+\frac{1}{2}}, y_n), \tag{4.11}$$

$$y_{n+1} = y_n + hf(t_{n+1}, x_{n+1}).$$

These rules are related to $\mathfrak{N}(t; h)$ by

$$M(t; h) = \mathfrak{N}\left(t; \frac{h}{2}\right), \tag{4.12}$$

$$T(t; h) = \mathfrak{N}\left(t + \frac{h}{2}; \frac{h}{2}\right) - \frac{h}{2}f\left(t, \mathfrak{N}\left(t; \frac{h}{2}\right)\right). \tag{4.13}$$

It follows directly from (4.12) that

$$M(t; h) \sim \sum_{m=0}^{\infty} e_m(t)\left(\frac{h}{2}\right)^{2m}, \qquad t \in I, h \in H,$$

and, by expanding the right side of (4.13) using (4.4–5), that

$$T(t; h) \sim \sum_{m=0}^{\infty} g_m(t) \left(\frac{h}{2}\right)^{2m}, \qquad t \in I, h \in H,$$

where

$$g_m(t) = \sum_{k=0}^{m} \frac{1}{(2k)!} f_{m-k}^{(2k)}(t).$$

Notice that now, by the initial conditions for the functions f_m, $g_m(a) = 0$, $m = 1, 2, \cdots$.

The rules $M(t; h)$ and $T(t; h)$ again provide two distinct h^2-expansions, and extrapolation for $\phi(t)$ is possible in either with an *arbitrary* sequence of N's. More generally one could consider the linear combination $\gamma M(t; h) + (1 - \gamma)T(t; h)$. Noting (2.12) it is natural to take $\gamma = \frac{1}{2}$ and thus to put

$$A(t; h) = \tfrac{1}{2}[M(t; h) + T(t; h)].$$

The rule $A(t; h)$ has the asymptotic expansion

$$A(t; h) \sim \sum_{m=0}^{\infty} [e_m(t) + g_m(t)] \left(\frac{h}{2}\right)^{2m}, \qquad t \in I, h \in H.$$

In particular

$$e_1(t) + g_1(t) = u_1(t) + \tfrac{1}{4}x''(t)$$

does not contain $v_1(t)$. This is reminiscent of the averaging procedure of Milne and Reynolds [17] for annihilating the leading "unstable" component of the discretization error.

Finally, the following observation guarantees the numerical stability of the (practical) step-by-step algorithms. If either of the rules M, T, or A is coupled with the Neville (Stoer) scheme using a fixed number of extrapolations per step h_0, then the entire process is a Runge-Kutta (one-step) method. The existence of the Stoer schemes at each step must be assumed in the latter case.

5. Special second order systems. Let f again satisfy the hypotheses of §3 and now let it be required to find $\phi(t)$ at a fixed point $t \in I$, where ϕ is the unique solution of the special second order system

$$(5.1) \qquad \begin{aligned} x(a) &= s, \qquad x'(a) = s', \\ x'' &= f(t, x), \end{aligned} \qquad t \in I.$$

The simplest linear k-step method of the form

$$\rho(E)x_n = h^2\sigma(E)f(t_n, x_n)$$

for the solution of (5.1) is the Störmer second order scheme:

$$x_{n+1} - 2x_n + x_{n-1} = h^2 f(t_n, x_n).$$

The simplest choice of starting values compatible with this method is

$$x_0 = s, \qquad x_1 = s + hs' + \frac{h}{2} f(a, s).$$

In its summed form, which reduces the accumulation of rounding errors [12, §6.4], the scheme takes a form similar to (4.11) but with one function evaluation per step:

$$\begin{aligned} x_0 &= s, \qquad y_0 = s' + \frac{h}{2} f(a, s), \\ x_{n+1} &= x_n + hy_n, \\ y_{n+1} &= y_n + hf(t_{n+1}, x_{n+1}). \end{aligned} \tag{5.2a}$$

The rules $S(t; h)$ and $S^*(t; h)$ are now defined by

$$\begin{aligned} S(t; h) &= x_N(h), \qquad Nh = t - a, \\ S^*(t; h) &= y_N(h) - \frac{h}{2} f(t, x_N(h)). \end{aligned} \tag{5.2b}$$

In order to state results similar to those of §4 let the functions $e_m(t)$, $t \in I$, be defined recursively by

$$e_0(t) \equiv \phi(t), \tag{5.3a}$$

and for $m = 1, 2, \cdots$ by

$$\begin{aligned} e_m(a) &= 0, \qquad e_m'(a) = -\sum_{k=1}^{m} \frac{1}{(2k+1)!} e_{m-k}^{(2k+1)}(a), \\ e_m'' &= J(t)e_m + a_m(t) + b_m(t), \qquad t \in I, \end{aligned} \tag{5.3b}$$

where

$$a_m(t) = -2 \sum_{k=1}^{m} \frac{1}{(2k+2)!} e_{m-k}^{(2k+2)}(t) \tag{5.3c}$$

and

$$\sum_{m=1}^{\infty} b_m(t) z^m \equiv \sum_{k=2}^{\infty} \frac{1}{k!} f^{(k)}(t, \phi(t)) \left(\sum_{m=1}^{\infty} e_m(t) z^m \right)^k. \tag{5.3d}$$

In addition put, for $m = 0, 1, \cdots,$

$$e_m^*(t) = \sum_{k=0}^{m} \frac{1}{(2k+1)!} e_{m-k}^{(2k+1)}(t), \tag{5.4}$$

and note that

$$e_0^*(t) \equiv \phi'(t).$$

THEOREM 5.1. *The rules $S(t; h)$ and $S^*(t; h)$ have the asymptotic expansions*

$$S(t; h) \sim \sum_{m=0}^{\infty} e_m(t)h^{2m}, \tag{5.5}$$

$$S^*(t; h) \sim \sum_{m=0}^{\infty} e_m^*(t)h^{2m}, \tag{5.6}$$

uniformly for $t \in I$ and steps $h \in H$.

The result (5.5) was recently stated by Mayers [16], but without explicit expressions for the functions $e_m(t)$. Theorem 5.1 is actually more satisfying than the corresponding results for first order systems. There is no fear of instability brought on by the numerical method. If instability exists it is normally inherent in the differential equation (5.1). The methods for special second order equations are usually justified by the fact that a saving can be achieved if one avoids computation of the derivative $\phi'(t)$. It is necessary to know $\phi'(t)$ for the step-by-step use of (5.2) coupled with extrapolation schemes. It is therefore noteworthy that an h^2-expansion can be obtained for its calculation with *no increase* in the number of evaluations of f.

Proof of Theorem 5.1. For $p \geqq 1$ and $t = t_n = a + nh$ let

$$\epsilon_n(h) \equiv x_n(h) - \phi(t) - \delta_n(h),$$

$$\delta_n(h) \equiv \sum_{m=1}^{p-1} e_m(t)h^{2m}.$$

To prove (5.5) it must be shown that $\epsilon_n(h) = O(h^{2p})$ uniformly for $t \in I$ and steps $h \in H$. This is known for $p = 1$ [12, Theorem 6.7]. Define the linear operator $\mathfrak{L}$ by

$$\mathfrak{L}\epsilon_n = \epsilon_{n+1} - 2\epsilon_n + \epsilon_{n-1} - h^2 J(t)\epsilon_n .$$

For $p > 1$ the required result will follow from

$$\epsilon_0(h) = 0, \qquad \epsilon_1(h) = O(h^{2p+1}), \tag{5.7a}$$

$$\mathfrak{L}\epsilon_n(h) = O(h^4 \, \| \, \epsilon_n(h) \, \|) + O(h^{2p+2}), \qquad t \in I, \ h \in H, \tag{5.7b}$$

by the result for $p = 1$ and $p - 1$ applications of [12, Lemma 6.3].

The verification of (5.7) is accomplished by showing, similar to the proof of Theorem 4.2, that

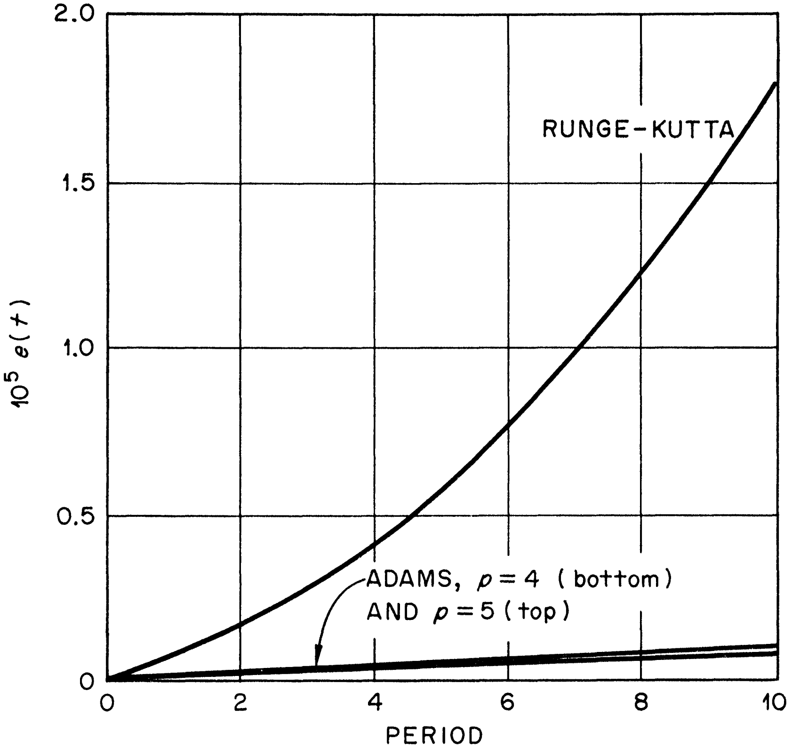

FIG. 1

$$-\epsilon_1(h) = \sum_{m=1}^{p-1}\left[e_m'(a) + \sum_{k=1}^{m}\frac{1}{(2k+1)!}e_{m-k}^{(2k+1)}(a)\right]h^{2m+1}$$

$$+\sum_{m=1}^{p-1}\left[\frac{1}{2}e_m''(a) + \sum_{k=1}^{m}\frac{1}{(2k+2)!}e_{m-k}^{(2k+2)}(a)\right]h^{2m+2} + O(h^{2p+1}), \qquad h \in H,$$

and

$$-\mathcal{L}\epsilon_n(h) = h^2\sum_{m=1}^{p-1}[e_m''(t) - J(t)e_m(t) - a_m(t) - b_m(t)]h^{2m}$$

$$+ O(h^4 \,\|\, \epsilon_n(h) \,\|) + O(h^{2p+2}), \quad t \in I, h \in H,$$

and then applying the definitions (5.3).

To prove (5.6) note that

$$S^*(t; h) = h^{-1}[S(t + h; h) - S(t; h)] - \frac{h}{2}f(t, S(t; h)),$$

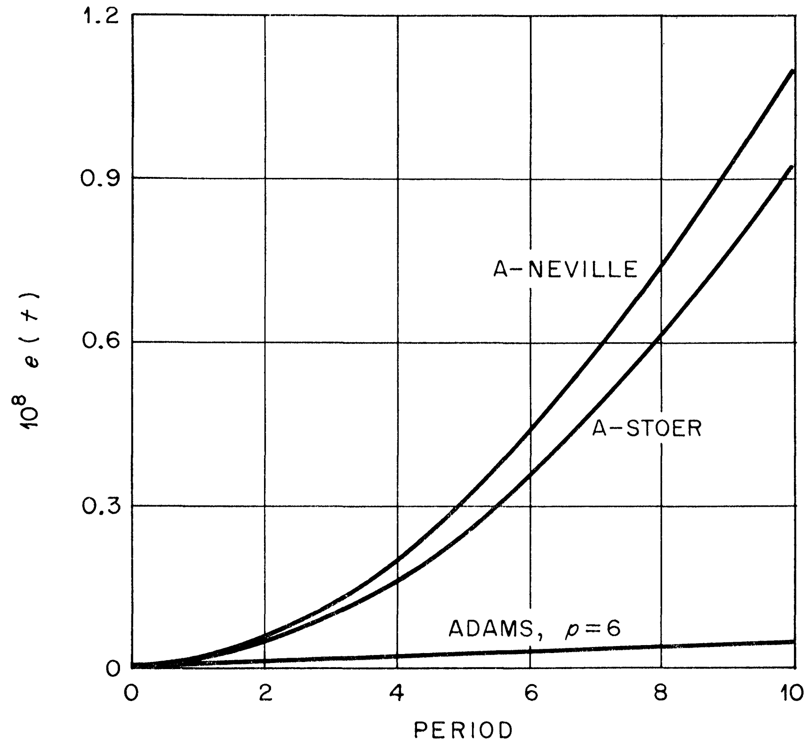

FIG. 2

and expand the right side using (5.3-5).

6. Numerical results. The restricted two-body problem

$$
\begin{aligned}
x(0) &= [1, 0]^T, \qquad x'(0) = [0, 1]^T, \\
x'' &= -\frac{x}{\| x \|^3}, \qquad 0 \leqq t \leqq 20\pi, \qquad (6.1)\\
\| x \| &= \text{sqrt } (x_1^2 + x_2^2),
\end{aligned}
$$

with exact solution

$$\phi(t) = [\cos t, \sin t]^T,$$

was solved numerically with the rules A and S, S^* coupled with the Neville and Stoer algorithms. To compare the A-schemes with some classical methods the formulation of (6.1) as a first order system was also solved by the Runge-Kutta method and Adams predictor-corrector pairs of order $p = 4, 5, 6$ with two corrections per step. The number of evaluations of f was approximately constant in this comparison.

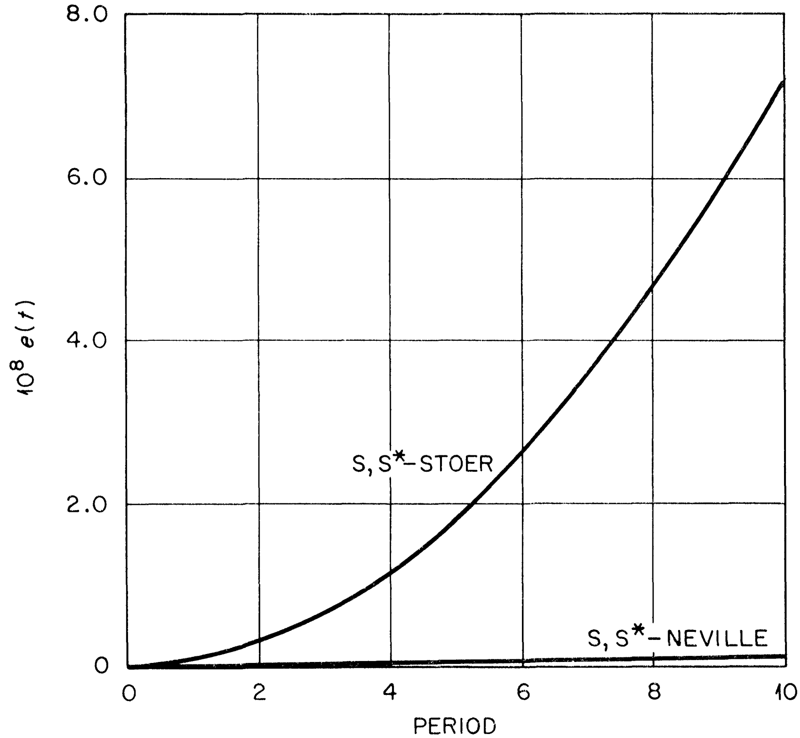

FIG. 3

The evaluations of f were accurate to 39 binary places; high precision was used in the remaining computations. The extrapolation schemes used the sequence (2.5) with $h_0 = \pi/3$, $\alpha = 1/\text{sqrt}\ (2)$, and six extrapolations per "global" step h_0. Figs. 1–3 show the results of these experiments. The error $e(t) = \| \tilde{x}(t) - \phi(t) \|$, where $\tilde{x}(t)$ is the numerical solution, is plotted as a function of the number of periods.

The error curves had roughly the same shape in each case; some appear linear due to the scale. The efficiency of the extrapolation algorithms is somewhat lower than the Adams sixth order method in this example. This standing can be improved by using higher precision and, perhaps, a slightly larger value of α. A similar comparison with seven extrapolations per step gave maximum errors of $\sim 2.10^{-11}$ for both the A-Neville scheme and the Adams sixth order method. The error was pure rounding error in these cases. It is interesting that the Neville algorithm gave better results, when coupled with S, S^*, than the Stoer algorithm. This does not appear to be a typical example however.

To test the effect of weak instability in the rule M, the linear system

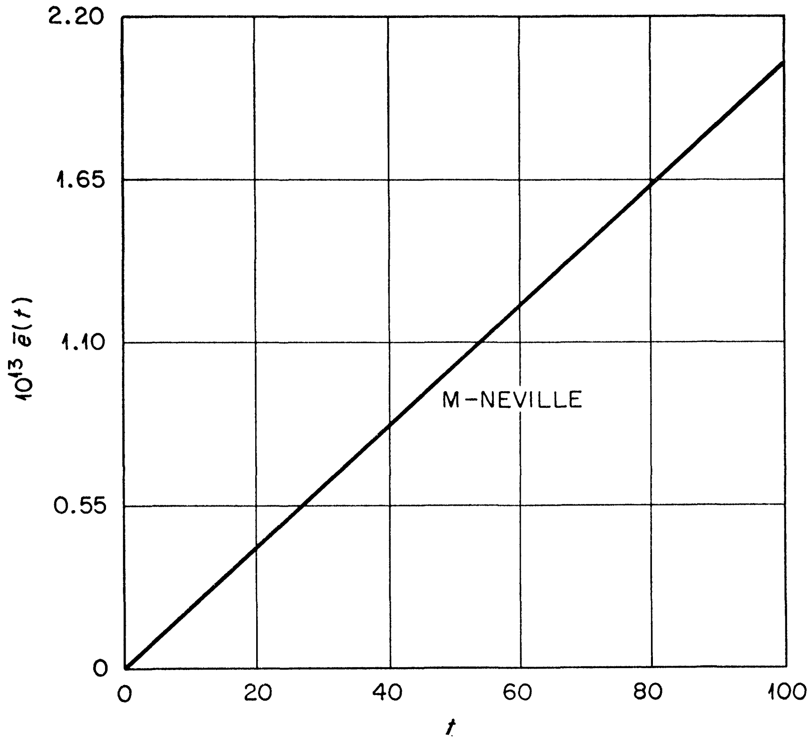

FIG. 4

$$x(0) = [0, 1]^T,$$

$$x' = Ax, \qquad 0 \leqq t \leqq 100, \qquad A = \begin{bmatrix} -1 & 1 \\ -1 & -1 \end{bmatrix},$$

with exact solution

$$\phi(t) = e^{-t}[\sin t, \cos t]^T,$$

was solved (in high precision) with the sequence $h(\frac{1}{2}^+)$, $h_0 = 1$, and six extrapolations per step. Fig. 4 shows the *relative* error $\bar{e}(t) = e^t \| \tilde{x}(t) - \phi(t) \|$ as a function of t.

In conclusion, it should be noted that the extrapolation algorithms provide good estimates of the "local error" and are extremely flexible with regard to variation of the step h_0.

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