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Introduction

By expanding the solution to the initial value problem

$$y' = f(t,y) \qquad y(t_0) = y_0 \tag{1.1a,b}$$

in a Taylor series about t_0, one obtains a local solution which is valid within its radius of convergence R_0. If the series is evaluated at t_1, where $t_1 < R_0$, one obtains an approximation to $y(t_1)$, and the solution may then be expanded in a new series about t_1. The solution may of course then be extended to the point t_2, and so forth, so that by a process of "analytic continuation" one obtains a piecewise polynomial solution to (1.1).

When the derivatives of y can be obtained cheaply, the method of Taylor series, or analytic continuation, offers several advantages over other methods. Foremost among these is that a Taylor series solution provides information that is not provided by other methods. This includes derivative information, local radius of convergence, and the location of poles in the complex plane. Another advantage is that both the stepsize and order can be easily changed, so that an optimal stepsize can always be chosen. Finally, Taylor series integration provides a piecewise continuous solution to the ODE, so that it is never necessary to interpolate at intermediate points.

Since analytic continuation is efficient only when high order derivatives can be obtained inexpensively, much effort has been made to develop recursive techniques that can generate the derivatives numerically. The first known attempt to incorporate recursion into the Taylor series method was by J.R. Airey in 1932 [1]. Miller was the first to employ a full recurrence scheme in which all series coefficients were calculated numerically, and the first to develop a systematic approach which was applicable to a class of differential equations [2,3]. Other early work includes that of Gibbons [4] and Moore [5], who developed programs that automatically generate the series coefficients for differential systems in canonical form. Other work concerning automated differentiation is that of Leavitt [6], Nikolaev [7], Barton *et. al.* [8,9], Norman [10], Kedem [11], Rall [12], Chang [13], Corliss and Chang [14], Irvine and Savageau [15], and Savageau and Voit [16].

Of the above, the most complete and systematic treatments of the Taylor series method are those of Barton, Willers, and Zahar [8,9], Chang [13,17,18] and Corliss and Chang [14], and Irvine and Savageau [15]. Barton *et.al.* were the first to develop and implement a general purpose algorithm that automatically reduces a given differential system to canonical form and generates the series coefficients without any previous manipulations by the user. Chang and Corliss developed a similar approach along with computer programs that are fully portable. Their programs also provide information on the location and order of primary singularities. Irvine and Savageau developed highly efficient series methods for differential equations that can be expressed in the form of an "S-system". Their approach obviates the need to generate problem-dependent source code for each new problem.

Corliss and Chang and Irvine and Savageau compared their codes with several standard ODE solvers on the problem set of Hull *et.al.* [19]. Compared to the IMSL routines DVERK (Runge-Kutta method) and DGEAR (variable order Adams method), Corliss and Chang report that their code was significantly faster for error tolerances in the range 10^{-9} to 10^{-12}. They conclude that the Taylor series method is superior to the variable order Adams method and the Runge-Kutta method when stringent accuracies are required and when solving small systems. Irvine and Savageau compared their method with two standard Runge-Kutta schemes, a variable order Adams method, and Gear's method. On an S-system from cellular biology, they report solution times that were significantly faster than all four methods for error tolerances ranging from 10^{-1} to 10^{-15}. In some cases, their code was faster by one or two orders of magnitude. On Hull's problem set, their results compared favorably both in terms of solution times and number of function evaluations. For small error tolerances, their code was up to 20 times faster. One concludes that the Taylor series method is indeed competitive with other methods, especially when high accuracies are required.

In this paper we propose an extension of the Taylor series method which improves its accuracy and stability while also increasing its range of applicability. The basic idea is to formulate the method as a generalized implicit method. Specifically, given an interval $[t_n, t_{n+1}]$, we consider a series solution to (1.1) which is expanded about the intermediate point $t_n + \mu h$, where h is the stepsize and μ is an arbitrary parameter called an expansion coefficient.

The main results of the paper are the following. (i) We derive the discretization error for a series solution to (1.1) which is expanded about the point $t_n + \mu h$. It is shown that a series of degree k has exactly k expansion coefficients which raise its order of accuracy. The increase is one order if k is odd, and two orders if k is even. For k odd, it will be seen that a class of Turan type, one-stage implicit Runge-Kutta methods are recovered [20]. (ii) We consider stability for the problem $y' = \lambda y$, $\mathrm{Re}(\lambda) < 0$, and identify several *A-stable* schemes. (iii) We show that, for all series of degree three or higher, local extrapolation can be used to increase accuracy by two additional orders. (iv) We discuss variable step schemes. (v) We present numerical results for a range of problems, including ODE's with a singular point and stiff systems. Our results indicate that implicit Taylor series methods are an effective integration tool for most problems.

Taylor Series of Degree One

We assume that $f(t, y)$ is a real-valued function which is analytic at the point (t_n, y_n), and that the problem

$$y' = f(t, y), \qquad y(t_n) = y_n, \tag{2.1a,b}$$

has a unique, continuous solution which can be expressed as a power series that converges for all t in the interval $|t - t_n| < R_n$. We denote the stepsize $t_{n+1} - t_n$ by h, where $h < R_n$.

A Taylor series of first degree expanded about t_n gives the equation

$$y(t_{n+1}) = y(t_n) + h\, f(t_n, y_n) + \frac{h^2}{2} f'(\xi_n, y(\xi_n)), \quad t_n < \xi_n < t_{n+1}, \tag{2.2}$$

from which one obtains Euler's method

$$y_{n+1} = y_n + h\, f(t_n, y_n) \tag{2.3}$$

and its associated discretization error $\frac{h^2}{2} f'(\xi_n, y(\xi_n)) := y''(\xi_n)$. The error may also be expressed by the expansion

$$e_{n+1} := y(t_{n+1}) - y_{n+1} = \frac{h^2}{2} f'_n + \frac{h^3}{6} f''_n + \frac{h^4}{24} f'''_n + \cdots \tag{2.4}$$

where $f'_n := f'(t_n, y_n)$, and similarly for f''_n and f'''_n.

If the series is expanded about t_{n+1}, one obtains the backward Euler method

$$y_{n+1} = y_n + h\, f(t_{n+1}, y_{n+1}), \tag{2.5}$$

where y_{n+1} must be obtained implicitly. By expanding $f(t_{n+1}, y_{n+1})$ in a Taylor series about (t_n, y_n), one derives from (2.5) the discretization error

$$e_{n+1} := y(t_{n+1}) - y_{n+1} = - \Big[\frac{h^2}{2} f'_n + \frac{h^3}{6} (2\, f''_n + 3\, \frac{\partial f_n}{\partial y} f'_n)$$

$$+ \frac{h^4}{24} (3\, f'''_n + 8\, \frac{\partial f_n}{\partial y} f''_n + 12\, \frac{\partial f'_n}{\partial y} f'_n) \Big] + O(h^5). \tag{2.6}$$

Both the forward and backward Euler methods provide a linear approximation to y on $I_n := [t_n, t_{n+1}]$. This approximation can be written

$$\underset{\sim}{y_n} = y_{n+\mu} + (t - t_{n+\mu})\, f(t_{n+\mu}, y_{n+\mu}), \qquad t_n \le t \le t_{n+1}, \tag{2.7}$$

where μ is zero or one, respectively.

If we define $t_{n+\mu} := t_n + \mu\, h$, where $0 \le \mu \le 1$, Eq. (2.7) becomes a generalized approximation to y on I_n. In this case the approximation will pass through the intermediate value $y_{n+\mu}$, which is unknown. By observing that $\underset{\sim}{y}_n$ must equal y_n when $t = t_n$, one can see that $y_{n+\mu}$ must be determined from

$$y_{n+\mu} \;=\; y_n \;+\; \mu\, h\, f(t_{n+\mu}, y_{n+\mu}). \tag{2.8a}$$

Note that this is just the backward Euler method for the partial step from t_n to $t_{n+\mu}$. Once $y_{n+\mu}$ is determined from (2.8a), one sets $t = t_{n+1}$, $\underset{\sim}{y}_n = y_{n+1}$ in (2.7) to obtain

$$y_{n+1} \;=\; y_{n+\mu} \;+\; (1-\mu)\, h\, f(t_{n+\mu}, y_{n+\mu}). \tag{2.8b}$$

One observes that this is just the forward Euler method for the partial step from $t_{n+\mu}$ to t_{n+1}. Thus, two steps are required to advance the solution to t_{n+1} - a backward Euler intermediate step followed by a forward Euler final step.

To determine an optimal expansion point $t_{n+\mu}$, one obtains the truncation error for (2.8). Since (2.8a) is the backward Euler method with stepsize $\mu\, h$, one uses (2.6) to obtain an expansion for $y_{n+\mu}$, which may then be substituted into (2.8b). One gets from (2.6),

$$\begin{aligned} y_{n+\mu} \;=\; & y_n \;+\; \mu\, h\, f_n \;+\; (\mu\, h)^2\, f_n' \;+\; \frac{(\mu\, h)^3}{2}\left(f_n'' + \frac{\partial f_n}{\partial y}\, f_n'\right) \\ & + \frac{(\mu\, h)^4}{6}\left(f_n''' \;+\; 2\,\frac{\partial f_n}{\partial y}\, f_n'' \;+\; 3\,\frac{\partial f_n'}{\partial y}\, f_n'\right) \;+\; O(h^5). \end{aligned} \tag{2.9}$$

Upon expanding $f(t_{n+\mu}, y_{n+\mu})$ about (t_n, y_n), and evaluating powers of $(y_{n+\mu} - y_n)$ by way of (2.9), one obtains from (2.8b)

$$\begin{aligned} y_{n+1} \;=\; & y_n \;+\; h\, f_n \;+\; \mu\, h^2\, f_n' \;+\; \mu^2\,\frac{h^3}{2}\left(f_n'' + \frac{\partial f_n}{\partial y}\, f_n'\right) \\ & + \mu^3\,\frac{h^4}{6}\left(f_n''' \;+\; 2\,\frac{\partial f_n}{\partial y}\, f_n'' \;+\; 3\,\frac{\partial f_n'}{\partial y}\, f_n'\right) \;+\; O(h^5). \end{aligned} \tag{2.10}$$

The error expansion for (2.8) is then

$$\begin{aligned} e_{n+1} \;:=\; y(t_{n+1}) \;-\; y_{n+1} \;=\; & (1-2\,\mu)\,\frac{h^2}{2}\, f_n' \;+\; \frac{h^3}{6}\left[(1-3\,\mu^2)\, f_n'' \;-\; 3\,\mu^2\,\frac{\partial f_n}{\partial y}\, f_n'\right] \\ & + \frac{h^4}{24}\left[(1 \;-\; 4\,\mu^3) f_n''' \;-\; \mu^3\left(8\,\frac{\partial f_n}{\partial y}\, f_n'' \;+\; 12\,\frac{\partial f_n'}{\partial y}\, f_n'\right)\right] \;+\; O(h^5). \end{aligned} \tag{2.11}$$

Taking $\mu = \frac{1}{2}$, the marching scheme becomes

$$y_{n+\frac{1}{2}} = y_n + \frac{h}{2} f(t_{n+\frac{1}{2}}, y_{n+\frac{1}{2}}) \tag{2.12a}$$

$$y_{n+1} = y_{n+\frac{1}{2}} + \frac{h}{2} f(t_{n+\frac{1}{2}}, y_{n+\frac{1}{2}}), \tag{2.12b}$$

with discretization error

$$e_{n+1} = \frac{h^3}{24}\left(f_n'' - 3\frac{\partial f_n}{\partial y} f_n'\right)$$

$$+ \frac{h^4}{48}\left(f_n''' - 2\frac{\partial f_n}{\partial y} f_n'' - 3\frac{\partial f_n'}{\partial y} f_n'\right) + O(h^5). \tag{2.13}$$

The choice $\mu = \frac{1}{2}$ thus leads to a second-order scheme. In view of the central expansion point $t_{n+\frac{1}{2}}$, we will refer to (2.12) as the "centered Euler method".

It should be noted that, corresponding to (2.12), the linear expansion (2.7) approximates $y(t)$ with an error at most equal to $\frac{h^2}{8}|f_n'| + O(h^3)$. This is one-fourth the error bound on (2.7) corresponding to the forward and backward Euler methods.

We should also mention that the explicit halfstep (2.12b) can be equivalently expressed as

$$y_{n+1} = y_n + h f(t_{n+\frac{1}{2}}, y_{n+\frac{1}{2}}). \tag{2.14}$$

When written in this form, it is clear that the centered Euler method is similar to the trapezoidal rule

$$y_{n+1} = y_n + \frac{h}{2}\left[f(t_n, y_n) + f(t_{n+1}, y_{n+1})\right]. \tag{2.15}$$

It is also similar to the one-stage Gauss implicit scheme [21], [22],

$$y_{n+1} = y_n + k_1 \tag{2.16a}$$

$$k_1 = h f(t_{n+\frac{1}{2}}, y_n + \tfrac{1}{2}k_1), \tag{2.16b}$$

which is equivalent to the implicit midpoint rule [22],

$$y_{n+1} = y_n + h f\left(t_{n+\frac{1}{2}}, \tfrac{1}{2}(y_n + y_{n+1})\right). \tag{2.17}$$

It can be shown in fact that the centered Euler method and the implicit midpoint rule are equivalent schemes. One can also show that the trapezoidal linear approximation to y on I_n,

$$y_T(t) = y_n + (t - t_n)\frac{f(t_n, y_n) + f(t_{n+1}, y_{n+1})}{2}, \tag{2.18}$$

approximates y with a maximum error equal to that of the centered Euler method, $\frac{h^2}{8}|f_n'| + O(h^3)$. One concludes that these three schemes offer nearly identical benefits over the forward and backward Euler methods.

Taylor Series of Degree Two

Analogous to Eq. (2.7), a Taylor series of second degree expanded about the point $t_{n+\mu}$ approximates y on I_n by

$$y_{\tilde{n}} \;=\; y_{n+\mu} \;+\; (t - t_{n+\mu})\, f(t_{n+\mu}, y_{n+\mu}) \;+\; \frac{(t - t_{n+\mu})^2}{2}\, f'(t_{n+\mu}, y_{n+\mu}). \qquad (3.1)$$

As in the previous section, the expansion coefficient μ defines a family of marching schemes. Choosing $\mu = 0$ and setting $t = t_{n+1}$, $y_{\tilde{n}} = y_{n+1}$, one obtains the Taylor series method of order two

$$y_{n+1} \;=\; y_n \;+\; h\, f(t_n, y_n) \;+\; \frac{h^2}{2}\, f'(t_n, y_n) \qquad (3.2)$$

with local error

$$e_{n+1} \;=\; \frac{h^3}{6}\, f_n'' \;+\; \frac{h^4}{24}\, f_n''' \;+\; \frac{h^5}{5!}\, f_n'''' \;+\; \cdots \qquad (3.3)$$

Similarly, choosing $\mu = 1$ and setting $t = t_n$, $y_{\tilde{n}} = y_n$, one obtains the implicit method

$$y_{n+1} \;=\; y_n \;+\; h\, f(t_{n+1}, y_{n+1}) \;-\; \frac{h^2}{2}\, f'(t_{n+1}, y_{n+1}). \qquad (3.4)$$

By expanding both $f(t_{n+1}, y_{n+1})$ and $f'(t_{n+1}, y_{n+1})$ in a Taylor series about (t_n, y_n), one derives from (3.4) the error expansion

$$\begin{aligned} e_{n+1} \;=&\; \frac{h^3}{6}\, f_n'' \;+\; \frac{h^4}{24}\,(3\, f_n''' \;+\; 4\, \frac{\partial f_n}{\partial y}\, f_n'') \\ &+\; \frac{h^5}{5!}\,(6\, f_n'''' \;+\; 15\, \frac{\partial f_n}{\partial y}\, f_n''' \;+\; 10\, \frac{\partial f_n'}{\partial y}\, f_n'') \;+\; O(h^6). \end{aligned} \qquad (3.5)$$

When $0 < \mu < 1$, (3.1) leads to a two-halfstep, implicit/explicit marching scheme, analogous to (2.8). Setting $t = t_n$, $y_{\tilde{n}} = y_n$, one obtains the implicit halfstep

$$y_{n+\mu} \;=\; y_n \;+\; \mu\, h\, f(t_{n+\mu}, y_{n+\mu}) \;-\; \frac{(\mu\, h)^2}{2}\, f'(t_{n+\mu}, y_{n+\mu}). \qquad (3.6a)$$

Setting $t = t_{n+1}$, $y_{\tilde{n}} = y_{n+1}$, one obtains the explicit halfstep

$$y_{n+1} \;=\; y_{n+\mu} \;+\; (1 - \mu)\, h\, f(t_{n+\mu}, y_{n+\mu}) \;+\; \frac{[(1 - \mu)\, h]^2}{2}\, f'(t_{n+\mu}, y_{n+\mu}). \qquad (3.6b)$$

An error expansion for (3.6) can be derived by proceeding as in the previous section. Utilizing the fact that (3.6a) is just (3.4) for the partial step $\mu\, h$, one obtains an expansion for $y_{n+\mu}$ by way of Eq. (3.5). One gets

$$y_{n+\mu} \;=\; y_n \;+\; \mu\, h\, f_n \;+\; \frac{(\mu\, h)^2}{2}\, f_n' \;-\; \frac{(\mu\, h)^4}{12}\, (f_n''' + 2\, \frac{\partial f_n}{\partial y}\, f_n'')$$

$$- \frac{(\mu h)^5}{24} \left(f_n'''' + 3 \frac{\partial f_n}{\partial y} f_n''' + 2 \frac{\partial f_n'}{\partial y} f_n'' \right) + O(h^6). \tag{3.7}$$

An expansion for y_{n+1} is then obtained from (3.6b) by expanding $f(t_{n+\mu}, y_{n+\mu})$ and $f'(t_{n+\mu}, y_{n+\mu})$ about (t_n, y_n), and evaluating powers of $(y_{n+\mu} - y_n)$ by way of (3.7). Retaining terms through $O(h^5)$, one finds that

$$\begin{aligned} y_{n+1} &= y_n + h f_n + \frac{h^2}{2} f_n' + 3\mu(1-\mu) \frac{h^3}{6} f_n'' \\ &\quad + \mu^2 \frac{h^4}{24} \left[(6 - 8\mu) f_n''' - 4\mu \frac{\partial f_n}{\partial y} f_n'' \right] \\ &\quad + \mu^3 \frac{h^5}{5!} \left[(10 - 15\mu) f_n'''' - 15\mu \frac{\partial f_n}{\partial y} f_n''' - 10 \frac{\partial f_n'}{\partial y} f_n'' \right] + O(h^6). \end{aligned} \tag{3.8}$$

Subtracting the left hand side of (3.8) from $y(t_{n+1})$ and the right hand side from the Taylor series expansion of $y(t_{n+1})$, one obtains

$$\begin{aligned} e_{n+1} &= (1 - 3\mu + 3\mu^2) \frac{h^3}{6} f_n'' + \frac{h^4}{24} \left[(1 - 6\mu^2 + 8\mu^3) f_n''' + 4\mu^3 \frac{\partial f_n}{\partial y} f_n'' \right] \\ &\quad + \frac{h^5}{5!} \left[(1 - 10\mu^3 + 15\mu^4) f_n'''' + 15\mu^4 \frac{\partial f_n}{\partial y} f_n''' + 10\mu^3 \frac{\partial f_n'}{\partial y} f_n'' \right] + O(h^6). \end{aligned} \tag{3.9}$$

Setting the leading coefficient to zero,

$$1 - 3\mu + 3\mu^2 = 0, \tag{3.10}$$

one finds

$$\mu = \frac{1}{2} \pm i \frac{\sqrt{3}}{6}, \tag{3.11}$$

so that the expansion point $t_{n+\mu} := t_n + \mu h$ must be moved into the complex plane. Upon substituting $\mu = \frac{1}{2} \pm i \frac{\sqrt{3}}{6}$ into (3.9), one obtains the complex truncation error

$$\begin{aligned} e_{n+1} &= \frac{h^5}{720} \left(f_n'''' - 5 \frac{\partial f_n}{\partial y} f_n''' \right) \\ &\quad \mp i \left[\frac{\sqrt{3}}{216} h^4 \left(f_n''' - 4 \frac{\partial f_n}{\partial y} f_n'' \right) + \frac{\sqrt{3}}{432} h^5 \left(f_n'''' - 3 \frac{\partial f_n}{\partial y} f_n''' - 4 \frac{\partial f_n'}{\partial y} f_n'' \right) \right]. \end{aligned} \tag{3.12}$$

The above expression is valid so long as f is analytic in a sufficiently large neighborhood of (t_n, y_n) in the complex plane.

Equation (3.12) shows that for a real-valued function f, the real truncation error is $O(h^5)$. This is two orders higher than for any other value of μ. We should note further that with μ defined as above, (3.6) becomes

$$y_{n+\mu} \;=\; \mathrm{Re}(y_n) \;+\; \mu\, h\, f(t_{n+\mu}, y_{n+\mu}) \;-\; \frac{(\mu\, h)^2}{2}\, f'(t_{n+\mu}, y_{n+\mu}) \tag{3.13a}$$

$$y_{n+1} \;=\; y_{n+\mu} \;+\; \bar{\mu}\, h\, f(t_{n+\mu}, y_{n+\mu}) \;+\; \frac{(\bar{\mu} h)^2}{2}\, f'(t_{n+\mu}, y_{n+\mu}), \tag{3.13b}$$

where $\bar{\mu}$ is the complex conjugate of μ. All operations in (3.13) must be performed in complex arithmetic, while the solution at each time level is the real part of y_n.

If μ is real, one can verify that $\mu = \frac{1}{2}$ minimizes the truncation error e_{n+1} at a value of $\frac{h^3}{24}\, f_n'' + O(h^4)$, in which case (3.6) becomes

$$y_{n+\frac{1}{2}} \;=\; y_n \;+\; \frac{h}{2}\, f(t_{n+\frac{1}{2}}, y_{n+\frac{1}{2}}) \;-\; \frac{h^2}{8}\, f'(t_{n+\frac{1}{2}}, y_{n+\frac{1}{2}}) \tag{3.14a}$$

$$y_{n+1} \;=\; y_{n+\frac{1}{2}} \;+\; \frac{h}{2}\, f(t_{n+\frac{1}{2}}, y_{n+\frac{1}{2}}) \;+\; \frac{h^2}{8}\, f'(t_{n+\frac{1}{2}}, y_{n+\frac{1}{2}}). \tag{3.14b}$$

It can also be shown that, corresponding to (3.14), the quadratic expansion (3.1) approximates y on I_n with a maximum error of $\frac{h^3}{24}\, |f_n''| + O(h^4)$. The corresponding error bound for both (3.2) and (3.4) is $\frac{h^3}{6}\, |f_n''| + O(h^4)$. As in the linear case, a centered expansion has a maximum error which is one-fourth that of an expansion around either endpoint. It should also be observed that, while (3.14) is only a second-order scheme, it provides a polynomial approximation to y on I_n whose accuracy is one order higher than that of (2.12).

Taylor Series of Arbitrary Degree

Let $f^{(k)}(t, y)$ denote the kth total derivative of f with respect to t, where $f^{(0)}(t, y) := f(t, y)$. A Taylor series approximation of degree k to the exact solution y on $I_n := [t_n, t_{n+1}]$ is

$$\underset{\sim}{y_n} \;=\; y_{n+\mu} \;+\; (t - t_{n+\mu})\, f(t_{n+\mu}, y_{n+\mu}) \;+\; \frac{(t - t_{n+\mu})^2}{2!}\, f'(t_{n+\mu}, y_{n+\mu})$$

$$+\; \frac{(t - t_{n+\mu})^3}{3!}\, f''(t_{n+\mu}, y_{n+\mu}) \;+\; \cdots \;+\; \frac{(t - t_{n+\mu})^k}{k!}\, f^{(k-1)}(t_{n+\mu}, y_{n+\mu}), \tag{4.1}$$

where $t_{n+\mu} := t_n + \mu\, h$ and $0 \le \mathrm{Re}\,(\mu) \le 1$. As shown in the two previous sections, the expansion coefficient μ defines a family of marching schemes.

Corresponding to $\mu = 0$, one obtains the explicit Taylor series method of order k,

$$y_{n+1} \;=\; y_n \;+\; h\, f(t_n, y_n) \;+\; \frac{h^2}{2!}\, f'(t_n, y_n) \;+\; \cdots \;+\; \frac{h^k}{k!}\, f^{(k-1)}(t_n, y_n). \tag{4.2}$$

Corresponding to $\mu = 1$, one obtains the implicit series method

$$y_{n+1} = y_n + h\, f(t_{n+1}, y_{n+1}) - \frac{h^2}{2!}\, f'(t_{n+1}, y_{n+1})$$

$$+ \frac{h^3}{3!}\, f''(t_{n+1}, y_{n+1}) - \cdots + \cdots + (-1)^{k-1}\, \frac{h^k}{k!}\, f^{(k-1)}(t_{n+1}, y_{n+1}). \tag{4.3}$$

When $0 < \mathrm{Re}\,(\mu) < 1$, one obtains a two-halfstep implicit/explicit marching scheme analogous to (2.8) and (3.6), where the implicit and explicit halfsteps are,

$$y_{n+\mu} = y_n + \mu\, h\, f(t_{n+\mu}, y_{n+\mu}) - \frac{(\mu\, h)^2}{2!}\, f'(t_{n+\mu}, y_{n+\mu})$$

$$+ \frac{(\mu\, h)^3}{3!}\, f''(t_{n+\mu}, y_{n+\mu}) - \cdots + \cdots + (-1)^{k-1}\, \frac{(\mu\, h)^k}{k!}\, f^{(k-1)}(t_{n+\mu}, y_{n+\mu}) \tag{4.4a}$$

$$y_{n+1} = y_{n+\mu} + (1-\mu)\, h\, f(t_{n+\mu}, y_{n+\mu}) + \frac{[(1-\mu)\, h]^2}{2!}\, f'(t_{n+\mu}, y_{n+\mu})$$

$$+ \frac{[(1-\mu)\, h]^3}{3!}\, f''(t_{n+\mu}, y_{n+\mu}) + \cdots + \frac{[(1-\mu)\, h]^k}{k!}\, f^{(k-1)}(t_{n+\mu}, y_{n+\mu}), \tag{4.4b}$$

respectively.

The local error of (4.2) is

$$e_{n+1}^{(k)} = \frac{h^{k+1}}{(k+1)!}\, f_n^{(k)} + \frac{h^{k+2}}{(k+2)!}\, f_n^{(k+1)} + \frac{h^{k+3}}{(k+3)!}\, f_n^{(k+2)} + \cdots \tag{4.5}$$

The truncation error for (4.3) and (4.4) can also be derived. Corresponding to (4.3), one obtains

$$e_{n+1}^{(k)} = (-1)^k \left\{ \frac{h^{k+1}}{(k+1)!}\, f_n^{(k)} + \frac{h^{k+2}}{(k+2)!} \left[(k+1)\, f_n^{(k+1)} + (k+2)\, \frac{\partial f_n}{\partial y}\, f_n^{(k)} \right] \right.$$

$$+ \frac{h^{k+3}}{(k+3)!} \left[\frac{(k+1)(k+2)}{2}\, f_n^{(k+2)} + (k+1)(k+3)\, \frac{\partial f_n}{\partial y}\, f_n^{(k+1)} \right.$$

$$\left. \left. + \frac{(k+2)(k+3)}{2}\, \frac{\partial f_n'}{\partial y}\, f_n^{(k)}) \right] \right\} + O(h^{k+4}), \tag{4.6}$$

for all $k \geq 2$. A proof is given in the Appendix. (The error for $k = 1$ is given by (2.6), and only differs from (4.6) in the last term.)

The discretization error for (4.4) can be derived in a two-step process. Recognizing that (4.4a) is equivalent to (4.3) with a stepsize of $\mu\, h$, one uses (4.6), with h replaced by $\mu\, h$, to obtain an expansion for $y_{n+\mu}$. For k odd, one gets

$$y^{(k)}_{n+\mu} = y_n + \mu\, h\, f_n + \frac{(\mu\, h)^2}{2!}\, f'_n + \cdots + \frac{(\mu\, h)^k}{k!}\, f^{(k-1)}_n \tag{4.7}$$

$$+ 2\, \frac{(\mu\, h)^{k+1}}{(k+1)!}\, f^{(k)}_n + \frac{(\mu\, h)^{k+2}}{(k+2)!} \left[(k+2)\, f^{(k+1)}_n + (k+2)\, \frac{\partial f_n}{\partial y}\, f^{(k)}_n \right]$$

$$+ \frac{(\mu\, h)^{k+3}}{(k+3)!} \left[\frac{k^2 + 3\,k + 4}{2}\, f^{(k+2)}_n + (k+1)\,(k+3)\, \frac{\partial f_n}{\partial y}\, f^{(k+1)}_n + \frac{(k+2)\,(k+3)}{2}\, \frac{\partial f'_n}{\partial y}\, f^{(k)}_n \right]$$

$$+ O(h^{k+4}),$$

and for k even, one obtains

$$y^{(k)}_{n+\mu} = y_n + \mu\, h\, f_n + \frac{(\mu\, h)^2}{2!}\, f'_n + \cdots + \frac{(\mu\, h)^k}{k!}\, f^{(k-1)}_n \tag{4.8}$$

$$- \frac{(\mu\, h)^{k+2}}{(k+2)!} \left[k\, f^{(k+1)}_n + (k+2)\, \frac{\partial f_n}{\partial y}\, f^{(k)}_n \right]$$

$$- \frac{(\mu\, h)^{k+3}}{(k+3)!} \left[\frac{k\,(k+3)}{2}\, f^{(k+2)}_n + (k+1)\,(k+3)\, \frac{\partial f_n}{\partial y}\, f^{(k+1)}_n + \frac{(k+2)\,(k+3)}{2}\, \frac{\partial f'_n}{\partial y}\, f^{(k)}_n \right]$$

$$+ O(h^{k+4}).$$

One then expands $f(t_{n+\mu}, y_{n+\mu})$ and its total derivatives in (4.4b) in a series about (t_n, y_n). Powers of $(y_{n+\mu} - y_n)$ that appear are evaluated by way of (4.7) for k odd and by (4.8) for k even. It can be shown that $y^{(k)}_{n+1}$ agrees with the Taylor series expansion for $y(t_{n+1})$ through terms of order k. The $O(h^{k+1})$ term is a function of μ, and for k is odd, is given by

$$\frac{h^{k+1}}{(k+1)!}\, f^{(k)}_n \left\{ 2\, \mu^{k+1} + \left[(k+1)\, \mu^k\, (1-\mu) \right. \right. \tag{4.9}$$

$$\left. \left. + \frac{(k+1)\, k}{2!}\, \mu^{k-1}\, (1-\mu)^2 + \frac{(k+1)\, k\, (k-1)}{3!}\, \mu^{k-2}\, (1-\mu)^3 + \cdots + (k+1)\, \mu\, (1-\mu)^k \right] \right\}$$

and for k even, is given by

$$\frac{h^{k+1}}{(k+1)!}\, f_n^{(k)} \Bigg\{ \Big[(k+1)\, \mu^k \, (1-\mu) \tag{4.10}$$

$$+ \frac{(k+1)\, k}{2!}\, \mu^{k-1} (1-\mu)^2 + \frac{(k+1)\, k\, (k-1)}{3!}\, \mu^{k-2} (1-\mu)^3 + \cdots + (k+1)\, \mu \, (1-\mu)^k \Big] \Bigg\}.$$

The sum in brackets in (4.9) and (4.10) can be simplified by making use of the following identity, which follows from the binomial theorem.

$$\mu^k + k\, \mu^{k-1} (1-\mu) + \frac{k\, (k-1)}{2!}\, \mu^{k-2} (1-\mu)^2 \tag{4.11}$$

$$+ \frac{k\, (k-1)\, (k-2)}{3!}\, \mu^{k-3} (1-\mu)^3 + \cdots + k\, \mu \, (1-\mu)^{k-1} + (1-\mu)^k \equiv 1.$$

Equation (4.11) holds for all $k \geq 0$.

Now (4.9) can be written

$$\frac{h^{k+1}}{(k+1)!}\, f_n^{(k)} \Bigg\{ \mu^{k+1} + \Big[\mu^{k+1} + (k+1)\, \mu^k \, (1-\mu) \tag{4.12}$$

$$+ \frac{(k+1)\, k}{2!}\, \mu^{k-1} (1-\mu)^2 + \frac{(k+1)\, k\, (k-1)}{3!}\, \mu^{k-2} (1-\mu)^3 + \cdots + (k+1)\, \mu \, (1-\mu)^k$$

$$+ (1-\mu)^{k+1} \Big] - (1-\mu)^{k+1} \Bigg\}.$$

It follows from (4.11) that (4.12) equals

$$\frac{h^{k+1}}{(k+1)!}\, f_n^{(k)} \Big[\mu^{k+1} - (1-\mu)^{k+1} + 1 \Big] \tag{4.13}$$

Similarly, one rewrites (4.10) as

$$\frac{h^{k+1}}{(k+1)!}\, f_n^{(k)} \Bigg\{ - \mu^{k+1} + \Big[\mu^{k+1} + (k+1)\, \mu^k \, (1-\mu) \tag{4.14}$$

$$+ \frac{(k+1)\, k}{2!}\, \mu^{k-1} (1-\mu)^2 + \frac{(k+1)\, k\, (k-1)}{3!}\, \mu^{k-2} (1-\mu)^3 + \cdots + (k+1)\, \mu \, (1-\mu)^k$$

$$+ (1-\mu)^{k+1} \Big] - (1-\mu)^{k+1} \Bigg\}$$

which equals

$$\frac{h^{k+1}}{(k+1)!}\, f_n^{(k)} \Big[1 \;-\; \mu^{k+1} \;-\; (1-\mu)^{k+1}\Big]. \tag{4.15}$$

The expansion for $y_{n+1}^{(k)}$ is then, for k odd or even,

$$y_{n+1}^{(k)} \;=\; y_n \;+\; h\, f_n \;+\; \frac{h^2}{2!}\, f_n' \;+\; \cdots \;+\; \frac{h^k}{k!}\, f_n^{(k-1)}$$

$$+\; \frac{h^{k+1}}{(k+1)!}\, f_n^{(k)} \Big[1 \;+\; (-1)^{k+1}\, \mu^{k+1} \;-\; (1-\mu)^{k+1}\Big] \;+\; O(h^{k+2}). \tag{4.16}$$

It follows that the discretization error of the marching scheme (4.4) is

$$e_{n+1}^{(k)} \;=\; \Big[(1-\mu)^{k+1} \;+\; (-1)^k\, \mu^{k+1}\Big]\, \frac{h^{k+1}}{(k+1)!}\, f_n^{(k)} \;+\; O(h^{k+2}). \tag{4.17}$$

Equation (4.17) is valid for $0 \le \mathrm{Re}\,(\mu) \le 1$, and for all $k \ge 1$.

One may also derive the higher order terms for $e_{n+1}^{(k)}$ in a manner similar to the above. The next two terms in the expansion are

$$\Bigg\{\Bigg[(1-\mu)^{k+1} \;+\; (k+1)\,\mu\,\big[\,(1-\mu)^{k+1} \;+\; (-1)^k \mu^{k+1}\big]\,\Bigg] f_n^{(k+1)}$$

$$+\; (-1)^k\,(k+2)\,\mu^{k+1}\,\frac{\partial f_n}{\partial y}\, f_n^{(k)}\Bigg\}\,\frac{h^{k+2}}{(k+2)!} \tag{4.18}$$

and

$$\Bigg\{\Bigg[(1-\mu)^{k+1}\,\big[\,(k+1)\,\mu \;+\; 1\big] \;+\; \frac{(k+2)\,(k+1)}{2}\,\mu^2\,\big[\,(1-\mu)^{k+1} \;+\; (-1)^k \mu^{k+1}\big]\,\Bigg] f_n^{(k+2)}$$

$$+\; (-1)^k\,(k+3)\,(k+1)\,\mu^{k+2}\,\frac{\partial f_n}{\partial y}\, f_n^{(k+1)} \tag{4.19}$$

$$+\; (-1)^k\,\frac{(k+3)\,(k+2)}{2}\,\mu^{k+1}\,\frac{\partial f_n'}{\partial y}\, f_n^{(k)}\Bigg\}\,\frac{h^{k+3}}{(k+3)!}.$$

From (4.17) it follows that the optimal expansion coefficients for a Taylor series method of degree k are the roots of the equation

$$(1-\mu)^{k+1} \;+\; (-1)^k\, \mu^{k+1} \;=\; 0, \tag{4.20}$$

or

$$(1-\mu)^{k+1} \;-\; \mu^{k+1} \;=\; 0 \quad \text{for } k \text{ odd}, \tag{4.21a}$$

and

$$(1-\mu)^{k+1} + \mu^{k+1} = 0 \quad \text{for } k \text{ even.} \tag{4.21b}$$

Since the left hand sides of (4.21a,b) are polynomials of degree k, each equation has at most k distinct roots. One can show that the k roots of (4.21a) are

$$\mu = \frac{1}{2} \pm i\,\frac{1}{2}\tan\left[\frac{(m-1)\,\pi}{k+1}\right] \qquad m = 1, 2, \cdots, \frac{k+1}{2} \tag{4.22a}$$

and the k roots of (4.21b) are

$$\mu = \frac{1}{2} \pm i\,\frac{1}{2}\tan\left[\frac{(m-\frac{1}{2})\,\pi}{k+1}\right] \qquad m = 1, 2, \cdots, \frac{k}{2}. \tag{4.22b}$$

Equation (4.21a) thus has one real root, $\mu = \frac{1}{2}$, while Eq. (4.21b) has no real roots.

Using (4.17) – (4.20), the discretization error corresponding to all μ defined by (4.22) is

$$\begin{aligned} e_{n+1}^{(k,m)} &= \frac{h^{k+2}}{(k+2)!}\left[(1-\mu)^{k+1} f_n^{(k+1)} + (-1)^k\,(k+2)\,\mu^{k+1}\,\frac{\partial f_n}{\partial y}\,f_n^{(k)}\right] \\ &+ \frac{h^{k+3}}{(k+3)!}\left[(1-\mu)^{k+1}\left[(k+1)\,\mu + 1\right] f_n^{(k+2)} + (-1)^k\,(k+3)\,(k+1)\,\mu^{k+2}\,\frac{\partial f_n}{\partial y}\,f_n^{(k+1)}\right. \\ &\left. + (-1)^k\,\frac{(k+3)\,(k+2)}{2}\,\mu^{k+1}\,\frac{\partial f_n'}{\partial y}\,f_n^{(k)}\right]. \end{aligned} \tag{4.23}$$

Equation (4.23) can be simplified by utilizing, from (4.20),

$$(1-\mu)^{k+1} = (-1)^{k+1}\,\mu^{k+1}. \tag{4.24}$$

One obtains

$$\begin{aligned} e_{n+1}^{(k,m)} &= (-1)^{k+1}\,\mu^{k+1}\left\{\frac{h^{k+2}}{(k+2)!}\left[f_n^{(k+1)} - (k+2)\,\frac{\partial f_n}{\partial y}\,f_n^{(k)}\right]\right. \\ &+ \frac{h^{k+3}}{(k+3)!}\left[\mu\,(k+1)\left[f_n^{(k+2)} - (k+3)\,\frac{\partial f_n}{\partial y}\,f_n^{(k+1)}\right]\right. \\ &\left.\left. + f_n^{(k+2)} - \frac{(k+3)\,(k+2)}{2}\,\frac{\partial f_n'}{\partial y}\,f_n^{(k)}\right]\right\} + O(h^{k+4}). \end{aligned} \tag{4.25}$$

Now if μ is written in polar form, the expression for $e_{n+1}^{(k,m)}$ can be simplified further. By defining θ according to

$$\theta = \pm\,\frac{(m-1)\,\pi}{k+1}, \qquad \text{for } m = 1, 2, \cdots, \frac{k+1}{2} \quad \text{for } k \text{ odd} \tag{4.26a}$$

and

$$\theta \; = \; \pm \, \frac{(m - \frac{1}{2})\,\pi}{k+1}, \qquad \text{for } m = 1, 2, \cdots, \frac{k}{2} \quad \text{for } k \text{ even} \tag{4.26b}$$

one can write

$$\mu \; = \; \frac{1}{2} \, \sec\theta \, e^{i\theta}. \tag{4.27}$$

One then obtains

$$\mu^{k+1} \; = \; \left(\frac{1}{2} \, \sec\theta\right)^{k+1} e^{i(k+1)\theta}. \tag{4.28}$$

It follows that for k odd,

$$\mu^{k+1} \; = \; (-1)^{m+1} \left(\frac{1}{2} \, \sec\theta\right)^{k+1}, \tag{4.29a}$$

and for k even,

$$\mu^{k+1} \; = \; i \, (-1)^{m+1} \, \mathrm{sgn}(\theta) \left(\frac{1}{2} \, \sec\theta\right)^{k+1}. \tag{4.29b}$$

It is significant that μ^{k+1} is pure real when k is odd and pure imaginary when k is even. An inspection of (4.25) shows that if f is a real-valued function and k is odd, the $O(h^{k+2})$ error term is real. On the other hand, if f is real and k is even, the $O(h^{k+2})$ error term is pure imaginary. Consequently, the real truncation error is $O(h^{k+2})$ when k is odd, and $O(h^{k+3})$ when k is even. One thus obtains to leading order, for all odd $k \geq 1$ and for f real,

$$e_{n+1}^{(k,m)} \; = \; (-1)^{k+m} \left(\frac{1}{2} \, \sec\theta\right)^{k+1} \frac{h^{k+2}}{(k+2)!} \left[f_n^{(k+1)} \; - \; (k+2) \, \frac{\partial f_n}{\partial y} \, f_n^{(k)} \right] \tag{4.30}$$

where θ and m are defined by (4.26a). For even k, one obtains

$$e_{n+1}^{(k,m)} \; = \tag{4.31}$$

$$(-1)^{k+m+1} \, \frac{k+1}{2} \, |\tan\theta| \left(\frac{1}{2} \, \sec\theta\right)^{k+1} \frac{h^{k+3}}{(k+3)!} \left[f_n^{(k+2)} \; - \; (k+3) \, \frac{\partial f_n}{\partial y} \, f_n^{(k+1)} \right]$$

where θ and m are defined by (4.26b).

It is thus clear that, corresponding to the expansion coefficients derived above, a Taylor series method can have an accuracy which is one or two orders higher than the classical case in which $\mu = 0$. It also turns out that, due to the special form of the truncation error in (4.30) and (4.31), the accuracy of the solution can be raised two additional orders by local extrapolation. We will return to this point later in the paper.

One can now simplify the marching scheme (4.4) for all μ defined by (4.22). Using the fact that

$$1 \; - \; \mu \; = \; \bar{\mu}, \tag{4.32}$$

(4.4) becomes

$$y_{n+\mu} = \mathrm{Re}\,(y_n) + \mu\, h\, f(t_{n+\mu}, y_{n+\mu}) - \frac{(\mu\, h)^2}{2!}\, f'(t_{n+\mu}, y_{n+\mu})$$

$$+ \frac{(\mu\, h)^3}{3!}\, f''(t_{n+\mu}, y_{n+\mu}) - \cdots + \cdots + (-1)^{k-1}\, \frac{(\mu\, h)^k}{k!}\, f^{(k-1)}(t_{n+\mu}, y_{n+\mu}) \tag{4.33a}$$

$$y_{n+1} = y_{n+\mu} + \bar{\mu}\, h\, f(t_{n+\mu}, y_{n+\mu}) + \frac{(\bar{\mu}\, h)^2}{2!}\, f'(t_{n+\mu}, y_{n+\mu})$$

$$+ \frac{(\bar{\mu}\, h)^3}{3!}\, f''(t_{n+\mu}, y_{n+\mu}) + \cdots + \frac{(\bar{\mu}\, h)^k}{k!}\, f^{(k-1)}(t_{n+\mu}, y_{n+\mu}). \tag{4.33b}$$

For the special case $\mu = \frac{1}{2}$, one has $\mu = \bar{\mu}$, so that (4.33) can be written

$$y_{n+\frac{1}{2}} = y_n + \frac{1}{2}\, h\, f(t_{n+\frac{1}{2}}, y_{n+\frac{1}{2}}) - \frac{1}{2^2}\, \frac{h^2}{2!}\, f'(t_{n+\frac{1}{2}}, y_{n+\frac{1}{2}})$$

$$+ \frac{1}{2^3}\, \frac{h^3}{3!}\, f''(t_{n+\frac{1}{2}}, y_{n+\frac{1}{2}}) - \cdots + \cdots + (-1)^{k-1}\, \frac{1}{2^k}\, \frac{h^k}{k!}\, f^{(k-1)}(t_{n+\frac{1}{2}}, y_{n+\frac{1}{2}}) \tag{4.34a}$$

$$y_{n+1} = y_n + h\, f(t_{n+\frac{1}{2}}, y_{n+\frac{1}{2}}) + \frac{1}{2^2}\, \frac{h^3}{3!}\, f''(t_{n+\frac{1}{2}}, y_{n+\frac{1}{2}})$$

$$+ \frac{1}{2^4}\, \frac{h^5}{5!}\, f^{(4)}(t_{n+\frac{1}{2}}, y_{n+\frac{1}{2}}) + \cdots + \left[\frac{1}{2^k} + (-1)^{k-1}\, \frac{1}{2^k}\right] \frac{h^k}{k!}\, f^{(k-1)}(t_{n+\frac{1}{2}}, y_{n+\frac{1}{2}}). \tag{4.34b}$$

Note that all odd-ordered derivatives have been eliminated in (4.34b).

Scheme (4.34) is equivalent to a class of Turan type, one-stage implicit Runge-Kutta methods [20]. However, unlike implicit Runge-Kutta methods, the implicit step (4.34a) only requires the solution of a single equation, instead of a system of k equations. This advantage becomes significant when k is much bigger than one.

From (4.30), the local error of the real marching scheme (4.34) is, for all odd k,

$$e_{n+1}^{(k)} = \frac{1}{2^{k+1}}\, \frac{h^{k+2}}{(k+2)!} \left[f_n^{(k+1)} - (k+2)\, \frac{\partial f_n}{\partial y}\, f_n^{(k)}\right] + O(h^{k+3}). \tag{4.35a}$$

For even k, one obtains from (4.17)

$$e_{n+1}^{(k)} = \frac{1}{2^k}\, \frac{h^{k+1}}{(k+1)!}\, f_n^{(k)} + O(h^{k+2}). \tag{4.35b}$$

One also derives, corresponding to $\mu = \frac{1}{2}$, the following error bounds on the polynomial approximate $\underset{\sim}{y}_n(t)$ defined by (4.1).

k odd:

$$|y(t) \;-\; \underset{\sim}{y}_n(t)| \;\leq\; \frac{1}{2^{k+1}}\,\frac{h^{k+1}}{(k+1)!}\,|f_n^{(k)}| \;+\; O(h^{k+2}), \qquad t_n \leq t \leq t_{n+1} \tag{4.36a}$$

k even:

$$|y(t) \;-\; \underset{\sim}{y}_n(t)| \;\leq\; \frac{1}{2^{k}}\,\frac{h^{k+1}}{(k+1)!}\,|f_n^{(k)}| \;+\; O(h^{k+2}), \qquad t_n \leq t \leq t_{n+1}. \tag{4.36b}$$

Compared to the corresponding error bounds for $\mu = 0$ and $\mu = 1$, (4.36a) is more accurate by a factor of 2^{k+1}, and (4.36b) is more accurate by a factor of 2^k.

Stability for $y' \;=\; \lambda\, y, \quad \mathbf{Re}\,(\lambda) \;<\; 0$

Applying the marching scheme (4.4) to

$$y' \;=\; \lambda\, y, \qquad y(t_0) = y_0 \tag{5.1}$$

one gets

$$y_{n+1} \;=\; y_n\; \frac{1 \;+\; (1-\mu)\,\lambda\, h \;+\; (1-\mu)^2\,\lambda^2\,\frac{h^2}{2!} \;+\; \cdots \;+\; (1-\mu)^k\,\lambda^k\,\frac{h^k}{k!}}{1 \;-\; \mu\,\lambda\, h \;+\; \mu^2\,\lambda^2\,\frac{h^2}{2!} \;-\; \cdots \;+\; \cdots \;+\; (-1)^k\mu^k\,\lambda^k\,\frac{h^k}{k!}}, \tag{5.2}$$

so that the discrete solution is

$$y_n \;=\; y_0\left[\frac{1 \;+\; (1-\mu)\,\lambda\, h \;+\; (1-\mu)^2\,\lambda^2\,\frac{h^2}{2!} \;+\; \cdots \;+\; (1-\mu)^k\,\lambda^k\,\frac{h^k}{k!}}{1 \;-\; \mu\,\lambda\, h \;+\; \mu^2\,\lambda^2\,\frac{h^2}{2!} \;-\; \cdots \;+\; \cdots \;+\; (-1)^k\mu^k\,\lambda^k\,\frac{h^k}{k!}}\right]^n. \tag{5.3a}$$

Equation (5.3a) is valid for all μ satisfying $0 \leq \mathrm{Re}\,(\mu) \leq 1$.

Since the exact solution to (5.1), $y(t) = y_0\, e^{\lambda(t-t_0)}$, tends to zero as t tends to infinity when Re $(\lambda) < 0$, it follows that the stability criterion is

$$\left|\frac{1 \;+\; (1-\mu)\,\lambda\, h \;+\; (1-\mu)^2\,\lambda^2\,\frac{h^2}{2!} \;+\; \cdots \;+\; (1-\mu)^k\,\lambda^k\,\frac{h^k}{k!}}{1 \;-\; \mu\,\lambda\, h \;+\; \mu^2\,\lambda^2\,\frac{h^2}{2!} \;-\; \cdots \;+\; \cdots \;+\; (-1)^k\mu^k\,\lambda^k\,\frac{h^k}{k!}}\right| \;<\; 1. \tag{5.3b}$$

We consider the three cases $\mu = 0$, $\mu = 1$, and $\mathrm{Re}\,(\mu) = \frac{1}{2}$, for which (5.3) simplifies as follows.

$\mu = 0:$

$$y_n = y_0 \left(1 + \lambda h + \lambda^2 \frac{h^2}{2!} + \cdots + \lambda^k \frac{h^k}{k!} \right)^n \tag{5.4a}$$

$$\left| 1 + \lambda h + \lambda^2 \frac{h^2}{2!} + \cdots + \lambda^k \frac{h^k}{k!} \right| < 1 \tag{5.4b}$$

$\mu = 1:$

$$y_n = \frac{y_0}{\left[1 - \lambda h + \lambda^2 \frac{h^2}{2!} - \cdots + \cdots + (-1)^k \lambda^k \frac{h^k}{k!} \right]^n}. \tag{5.5a}$$

$$\left| 1 - \lambda h + \lambda^2 \frac{h^2}{2!} - \cdots + \cdots + (-1)^k \lambda^k \frac{h^k}{k!} \right| > 1 \tag{5.5b}$$

$\mathrm{Re}(\mu) = \frac{1}{2}:$

$$y_n = y_0 \left[\frac{1 + \bar{\mu} \lambda h + \bar{\mu}^2 \lambda^2 \frac{h^2}{2!} + \cdots + \bar{\mu}^k \lambda^k \frac{h^k}{k!}}{1 - \mu \lambda h + \mu^2 \lambda^2 \frac{h^2}{2!} - \cdots + \cdots + (-1)^k \mu^k \lambda^k \frac{h^k}{k!}} \right]^n \tag{5.6a}$$

$$\left| \frac{1 + \bar{\mu} \lambda h + \bar{\mu}^2 \lambda^2 \frac{h^2}{2!} + \cdots + \bar{\mu}^k \lambda^k \frac{h^k}{k!}}{1 - \mu \lambda h + \mu^2 \lambda^2 \frac{h^2}{2!} - \cdots + \cdots + (-1)^k \mu^k \lambda^k \frac{h^k}{k!}} \right| < 1 \tag{5.6b}$$

Degree-1 Taylor Series

Letting $\lambda h = w = u + i v$, where $u < 0$, the stability criterion for Euler's method is

$$|1 + w|^2 = (1 + u)^2 + v^2 < 1. \tag{5.7a}$$

The above inequality describes the set of points inside a circle of radius one centered at the point (-1,0) in the complex λh plane. For real λ, (5.7a) simplifies to

$$h < \frac{2}{-\lambda}. \tag{5.7b}$$

From (5.5b), the stability requirement of the backward Euler method is

$$|1 - w|^2 = (1 - u)^2 + v^2 > 1, \tag{5.8}$$

which is clearly satisfied for all negative u. The backward Euler solution thus tends to zero and remains stable for any fixed $h > 0$. Schemes which possess this property for problem (5.1) are said to be *A-stable* [23],[24].

From (5.6b), the stability requirement of the centered Euler method is

$$\left| \frac{1 + \bar{\mu} w}{1 - \mu w} \right|^2 < 1, \tag{5.9}$$

where $\mu = \bar{\mu} = \frac{1}{2}$. Since the centered Euler solution

$$y_n = y_0 \left(\frac{1 + \lambda \frac{h}{2}}{1 - \lambda \frac{h}{2}} \right)^n \tag{5.10}$$

is identical to that of the trapezoidal rule (which is known to be A-stable), it follows that the centered Euler method is also A-stable. (It should be noted that Dahlquist [25] has shown that the trapezoidal rule is the most accurate, A-stable scheme from the general class of linear multistep methods. The centered Euler method is, of course, a Taylor series method and therefore not in the same class. However, both methods give the same solution to $y' = \lambda y$.)

Degree-2 Taylor Series

The explicit stability requirement (5.4b) is

$$\left| 1 + w + \frac{w^2}{2} \right|^2 < 1, \tag{5.11a}$$

which reduces to

$$2u + 2u^2 + u(u^2 + v^2) + \frac{1}{4}(u^2 + v^2)^2 < 0. \tag{5.11b}$$

The above inequality is satisfied for all (u, v) such that

$$-2 < u < 0 \tag{5.12a}$$

$$|v| < \sqrt{2\sqrt{-u(u+2)} - u(u+2)}. \tag{5.12b}$$

See Figure 1.

The fully implicit stability criterion is

$$\left| 1 - w + \frac{w^2}{2} \right|^2 > 1, \tag{5.13a}$$

or

$$2u - 2u^2 + u(u^2 + v^2) - \frac{1}{4}(u^2 + v^2)^2 < 0. \tag{5.13b}$$

Since (5.13b) is satisfied for all $u < 0$, an implicit Taylor series of degree two is A-stable.

Stability requirement (5.6b) is

$$\left| \frac{1 + \bar{\mu} w + \bar{\mu}^2 \frac{w^2}{2}}{1 - \mu w + \mu^2 \frac{w^2}{2}} \right| < 1. \tag{5.14a}$$

Letting $\mu_i := \mathrm{Im}(\mu)$, it can be shown that (5.14a) holds if

$$u \left[2 + 4 \mu_i v + \left(\frac{1}{4} + \mu_i^2\right) \left(u^2 + v^2\right) \right] < 0. \tag{5.14b}$$

Inequality (5.14b) is clearly satisfied for all negative u when $\mu_i = 0$. For $\mu_i = \pm \frac{\sqrt{3}}{6}$, corresponding to (3.12), (5.14b) can be written

$$u \left[1 + \frac{u^2}{3} + \left(\frac{\sqrt{3}}{3} v \pm 1\right)^2 \right] < 0, \tag{5.15}$$

so that a degree-two series is A-stable for both $\mu = \frac{1}{2}$ and $\mu = \frac{1}{2} \pm i \frac{\sqrt{3}}{6}$.

Degree-3 Taylor Series

Proceeding as above, one derives the following stability constraints for Taylor series of degree three.

$\mu = 0:$

$$\begin{aligned} 2u + 2u^2 + \frac{4}{3} u^3 + \frac{1}{3} (u^4 - v^4) + \frac{1}{4} (u^2 + v^2)^2 \\ + \frac{1}{6} u (u^2 + v^2)^2 + \frac{1}{36} (u^2 + v^2)^3 < 0 \end{aligned} \tag{5.16}$$

$\mu = 1:$

$$\begin{aligned} 2u - 2u^2 + \frac{4}{3} u^3 - \frac{1}{3} (u^4 - v^4) - \frac{1}{4} (u^2 + v^2)^2 \\ + \frac{1}{6} u (u^2 + v^2)^2 - \frac{1}{36} (u^2 + v^2)^3 < 0 \end{aligned} \tag{5.17}$$

$\mu = \frac{1}{2} + i \mu_i:$

$$\begin{aligned} u \Big[2 + 4 \mu_i v + \frac{u^2}{3} + 4 \mu_i^2 v^2 + \frac{1}{6} \mu_i^2 u^2 v^2 + \frac{1}{3} \left(\frac{u^2}{4} + \mu_i^2 v^2\right) \left(\frac{v^2}{4} + \mu_i^2 u^2\right) \\ + \frac{4}{3} \mu_i v (u^2 + v^2) \left(\frac{1}{4} + \mu_i^2\right) + \frac{1}{6} (u^4 + v^4) \left(\frac{1}{16} + \mu_i^4\right) \Big] < 0 \end{aligned} \tag{5.18}$$

Because of the complexity of the above expressions, direct analysis is difficult. However, one can determine numerically that, corresponding to (5.16), an explicit series of degree three has the stability region shown in Figure 2. One can also show that near $v = \pm \sqrt{3}$, (5.17) is *not* satisfied as $u \to 0^-$, so that a degree-three, fully implicit series is not A-stable. See Figure 3.

Corresponding to (5.18), one considers stability for $\mu_i = 0$ and $\mu_i = \pm \frac{1}{2}$. (See (4.22a).) For $\mu_i = 0$, one can see directly that (5.18) is always satisfied when u is negative, so that a degree-three series is A-stable for $\mu = \frac{1}{2}$. However, for $\mu_i = \pm \frac{1}{2}$, one can show that (5.18) is not satisfied for all negative u. When $\mu_i = + \frac{1}{2}$, one obtains the instability region

$$- \sqrt{4\sqrt{-(v + 2)} - (v + 2)^2} \leq u < 0 \tag{5.19a}$$

$$-4.5198421 \leq v \leq -2, \tag{5.19b}$$

and when $\mu_i = -\frac{1}{2}$, one obtains

$$- \sqrt{4\sqrt{v - 2} - (v - 2)^2} \leq u < 0 \tag{5.20a}$$

$$2 \leq v \leq 4.5198421. \tag{5.20b}$$

See Figure 4.

Degree-4 Taylor Series

For Taylor series of degree four, one must rely primarily on numerical means to determine stability. We obtained the results shown in Figures 5 and 6 for explicit ($\mu = 0$) and fully implicit ($\mu = 1$) series, respectively. On the other hand, it is possible to show rigorously that, for $\mu = \frac{1}{2}$, the degree-four series is A-stable. However, corresponding to the two complex pairs $\mu = \frac{1}{2} \pm i\,\frac{1}{2}\tan\frac{\pi}{10}$ and $\mu = \frac{1}{2} \pm i\,\frac{1}{2}\tan\frac{3\pi}{10}$ defined by (4.22b), the degree-four series is not A-stable. See Figure 7.

Summary of A-Stable Taylor Series

To the best of our knowledge, there are no A-stable Taylor series of the form (4.4) with degree higher than four. (There are, however, A-stable schemes which use derivatives of arbitrarily high order [26],[27].) Table I summarizes the A-stable Taylor series identified in this section.

Taylor Series	Expansion Coefficient	Order of Accuracy
Degree-1	$\mu = 1$ (Backward Euler)	1st Order
	$\mu = \frac{1}{2}$ (Centered Euler)	2nd Order
Degree-2	$\mu = 1$	2nd Order
	$\mu = \frac{1}{2}$	2nd Order
	$\mu = \frac{1}{2} \pm i\frac{\sqrt{3}}{6}$	4th Order
Degree-3	$\mu = \frac{1}{2}$	4th Order
Degree-4	$\mu = \frac{1}{2}$	4th Order

Table I A-Stable Taylor series with their orders of accuracy.

Numerical Results - Uniform Stepsize

Our main objectives in this section are to verify the order-of-accuracy results presented earlier in the paper and to introduce extrapolation schemes for Taylor series of degree three and higher. We also discuss some details concerning the numerical implementation of the marching scheme (4.33). For a set of model problems, we consider Problems A1 - A5 from Hull *et. al.* [19], which are shown below.

Problem	ODE	Initial Condition	Exact Solution
1.	$y' = -y$	$y(0) = 1$	$y = e^{-t}$
2.	$y' = -\dfrac{y^3}{2}$	$y(0) = 1$	$y = \dfrac{1}{\sqrt{t+1}}$
3.	$y' = y \cos t$	$y(0) = 1$	$y = e^{\sin t}$
4.	$y' = \dfrac{y}{4}(1 - \dfrac{y}{20})$	$y(0) = 1$	$y = \dfrac{20}{1 + 19e^{-t/4}}$
5.	$y' = \dfrac{y-t}{y+t}$	$y(0) = 4$	$r = 4e^{\pi/2}e^{-\theta}$, $t = r\cos\theta$, $y = r\sin\theta$

Degree-1 Taylor Series

Corresponding to $k = 1$ and $\mu = \frac{1}{2}$, (4.33) becomes the centered Euler method (2.12a,b)

$$y_{n+\frac{1}{2}} = y_n + \frac{h}{2} f(t_{n+\frac{1}{2}}, y_{n+\frac{1}{2}})$$

$$y_{n+1} = y_{n+\frac{1}{2}} + \frac{h}{2} f(t_{n+\frac{1}{2}}, y_{n+\frac{1}{2}}).$$

For nonlinear f, the implicit halfstep (2.12a) must be solved by iteration. One can iterate on (2.12a) directly using corrector iteration,

$$y^{(l)}_{n+\frac{1}{2}} = y_n + \frac{h}{2} f(t_{n+\frac{1}{2}}, y^{(l-1)}_{n+\frac{1}{2}}), \tag{6.1}$$

where $y^{(0)}_{n+\frac{1}{2}} = y_n$. One can alternatively use Newton iteration,

$$y^{(l)}_{n+\frac{1}{2}} = y^{(l-1)}_{n+\frac{1}{2}} - \frac{y^{(l-1)}_{n+\frac{1}{2}} - \frac{h}{2}\, f\big(t_{n+\frac{1}{2}}, y^{(l-1)}_{n+\frac{1}{2}}\big) - y_n}{1 - \frac{h}{2}\,\frac{\partial f}{\partial y}\big(t_{n+\frac{1}{2}}, y^{(l-1)}_{n+\frac{1}{2}}\big)}. \tag{6.2}$$

For each method, the computational work per step depends on the number of iterations M required to solve (2.12a). See Tables II and III. Corresponding results for the implicit midpoint rule and trapezoidal rule are also shown for comparison.

We solved Problems 1 - 5 on the interval [0,20], with stepsize $h = 0.5$, 0.25, 0.125, ... Figure 8 shows the reduction of numerical error with stepsize. The corresponding orders of accuracy are shown in Table IV. All calculations were performed in double precision FORTRAN 77 on a Dell Dimension XPS R400 computer running under the LINUX operating system.

Operation	Centered Euler	Implicit Midpoint	Trapezoidal
Function Evaluations	M + 1	M	M + 1
Additions and Subtractions	M + 1	2 M	2 M
Multiplications	M + 1	2 M	M
Divisions	0	0	0

Table II   Computational Work Per Step – Corrector Method

Operation	Centered Euler	Implicit Midpoint	Trapezoidal
Function Evaluations	2 M + 1	2 M	2 M + 1
Additions and Subtractions	4 M + 1	5 M	5 M
Multiplications	2 M + 1	3 M	2 M
Divisions	M	M	M

Table III   Computational Work Per Step – Newton's Method

	Problem:				
	1	2	3	4	5
Method					
Centered Euler	2.00	1.98	2.02	1.99	2.06
Trapezoidal Rule	2.00	2.01	2.00	2.00	2.02
Implicit Midpoint	2.00	2.00	1.95	2.00	1.98

Table IV Numerical order of accuracy for Problems 1 - 5.

Degree-2 Taylor Series

Setting $k = 2$ and $\mu = \frac{1}{2} \pm i\,\frac{1}{2}\tan\frac{\pi}{6} = \frac{1}{2} \pm i\,\frac{\sqrt{3}}{6}$ in (4.33), one recovers the marching scheme (3.13a,b)

$$y_{n+\mu} = \mathrm{Re}\,(y_n) + \mu\,h\,f(t_{n+\mu}, y_{n+\mu}) - \frac{(\mu\,h)^2}{2}\,f'(t_{n+\mu}, y_{n+\mu})$$

$$y_{n+1} = y_{n+\mu} + \bar{\mu}\,h\,f(t_{n+\mu}, y_{n+\mu}) + \frac{(\bar{\mu}h)^2}{2}\,f'(t_{n+\mu}, y_{n+\mu}),$$

where the expansion point $t_{n+\mu} := t_n + \mu\,h$ is in the complex plane. Taking the "plus" sign for μ, the integration path takes the form shown in Figure 9.

Analogous to (6.1), corrector iteration for (3.13a) is given by

$$y_{n+\mu}^{(l)} = \mathrm{Re}\,(y_n) + \mu\,h\,f(t_{n+\mu}, y_{n+\mu}^{(l-1)}) - \frac{(\mu\,h)^2}{2}\,f'(t_{n+\mu}, y_{n+\mu}^{(l-1)}) \tag{6.3}$$

where $y_{n+\mu}^{(0)} = \mathrm{Re}(y_n)$. Similarly, Newton iteration for (3.13a) is

$$y_{n+\mu}^{(l)} = y_{n+\mu}^{(l-1)} - \frac{y_{n+\mu}^{(l-1)} - \mu\,h\,f\big(t_{n+\mu}, y_{n+\mu}^{(l-1)}\big) + \frac{(\mu\,h)^2}{2}\,f'\big(t_{n+\mu}, y_{n+\mu}^{(l-1)}\big) - \mathrm{Re}(y_n)}{1 - \mu\,h\,\frac{\partial f}{\partial y}\big(t_{n+\mu}, y_{n+\mu}^{(l-1)}\big) + \frac{(\mu\,h)^2}{2}\,\frac{\partial f'}{\partial y}\big(t_{n+\mu}, y_{n+\mu}^{(l-1)}\big)}. \tag{6.4}$$

Letting M denote the number of iterations required to solve (3.13a), the work per step is shown in Table V, where all operations must be performed in complex arithmetic. Note that the evaluation of $\frac{\partial f}{\partial y}$ in the denominator of (6.4) is not counted as a function evaluation, since it is part of the evaluation of f' in the numerator.

Application of the degree-2 Taylor series to Problems 1 - 5 on the interval [0,20] produced the error reduction results shown in Figure 10. Table VI shows the corresponding orders of accuracy.

Operation	Corrector Iteration	Newton Iteration
Function Evaluations	2 M + 2	3 M + 2
Additions and Subtractions	2 M + 2	6 M + 2
Multiplications	2 M + 2	4 M + 2
Divisions	0	M

Table V Computational work per step for a degree-2 Taylor series with $\mu = \frac{1}{2} \pm i\frac{\sqrt{3}}{6}$.

	Problem: 1	2	3	4	5
Expansion Coefficient					
$\mu = \frac{1}{2} + i\frac{\sqrt{3}}{6}$	4.04	3.96	4.12	3.97	4.23

Table VI Numerical order of accuracy for Problems 1 - 5 using a degree-2 Taylor series.

Degree-3 Taylor Series

From (4.22a) and (4.30), the marching scheme (4.33) is fourth-order-accurate when $k = 3$ and

$$\mu = \frac{1}{2} \tag{6.5}$$

or

$$\mu = \frac{1}{2} \pm i\,\frac{1}{2}. \tag{6.6}$$

Since $\mu = \frac{1}{2}$ is real and has the smallest truncation error, it is the preferred expansion coefficient.

The degree-3 Taylor series can be implemented using corrector or Newton iteration, analogous to (6.3) and (6.4), respectively. The work per step is shown in Table VII.

We now show that one can construct an extrapolation scheme using (6.5) - (6.6) which is sixth-order-accurate. Let $y_{n+1}^{(3,1)}$ denote the numerical solution at t_{n+1} corresponding to $\mu = \frac{1}{2}$, and let

$$e_{n+1}^{(3,1)} := y(t_{n+1}) - y_{n+1}^{(3,1)} \tag{6.7}$$

denote its truncation error. Similarly, let $y_{n+1}^{(3,2)}$ denote the numerical solution at t_{n+1} corresponding to $\mu = \frac{1}{2} + i\,\frac{1}{2}$, and let

$$e_{n+1}^{(3,2)} := y(t_{n+1}) - y_{n+1}^{(3,2)}. \tag{6.8}$$

Then one can see from (4.25) and (4.29a) that for a real-valued function f, $e_{n+1}^{(3,1)}$ and the real part of $e_{n+1}^{(3,2)}$ are related according to

$$\mathrm{Re}\Big(e_{n+1}^{(3,2)}\Big) = -4\,e_{n+1}^{(3,1)} + O(h^7). \tag{6.9}$$

Taking the real part of (6.8) and using (6.9), one gets

$$-4\,e_{n+1}^{(3,1)} + O(h^7) = y(t_{n+1}) - \mathrm{Re}\Big(y_{n+1}^{(3,2)}\Big). \tag{6.10}$$

Multiplying (6.7) by $\frac{4}{5}$ and (6.10) by $\frac{1}{5}$ and then adding the resulting equations and rearranging, one obtains

$$\frac{4}{5}\,y_{n+1}^{(3,1)} + \frac{1}{5}\,\mathrm{Re}\Big(y_{n+1}^{(3,2)}\Big) = y(t_{n+1}) + O(h^7). \tag{6.11}$$

The extrapolated solution

$$y_{n+1}^{(3,e)} := \frac{4}{5}\,y_{n+1}^{(3,1)} + \frac{1}{5}\,\mathrm{Re}\Big(y_{n+1}^{(3,2)}\Big) \tag{6.12}$$

is thus sixth-order-accurate.

In Figure 11 we show the stability region of the above extrapolation for problem (5.1). Figure 12 presents error reduction results for Problems 1 - 5 for $\mu = \frac{1}{2}$, $\mu = \frac{1}{2} + i\,\frac{1}{2}$, and extrapolation. The numerical orders of accuracy are shown in Table VIII.

Operation	Corrector Iteration	Newton Iteration
Function Evaluations	3 M + 3	4 M + 3
Additions and Subtractions	3 M + 3	8 M + 3
Multiplications	3 M + 3	6 M + 3
Divisions	0	M

Table VII Computational work per step for a degree-3 Taylor series with $\mu = \frac{1}{2}$ or $\mu = \frac{1}{2} \pm i\,\frac{1}{2}$.

Expansion Coefficient	Problem: 1	2	3	4	5
$\mu = \frac{1}{2}$	3.99	3.98	4.01	3.99	4.04
$\mu = \frac{1}{2} + i\,\frac{1}{2}$	4.01	3.91	4.02	3.97	3.94
extrapolation	6.11	5.89	6.03	6.02	6.20

Table VIII Numerical order of accuracy for Problems 1 - 5 using a degree-3 Taylor series.

Degree-4 Taylor Series

From (4.22b), one obtains the expansion coefficients

$$\mu = \frac{1}{2} \pm i\,\frac{1}{2}\,\tan\frac{\pi}{10} \tag{6.13}$$

and

$$\mu = \frac{1}{2} \pm i\,\frac{1}{2}\,\tan\frac{3\,\pi}{10}, \tag{6.14}$$

for which (4.33) is sixth-order-accurate. One can verify from (4.31) that (6.13) has a truncation error which is about 47 times smaller than that of (6.14).

Using a corrector or Newton iteration implementation, the degree-4 Taylor series requires the work per step shown in Table IX.

As in the previous section, extrapolation can be used to raise the accuracy of the degree-4 Taylor series by two additional orders. Rather than go through the details, we simply state the results.

Let $y_{n+1}^{(4,1)}$ denote the discrete solution at t_{n+1} when $\mu = \frac{1}{2} + i\,\frac{1}{2}\,\tan\frac{\pi}{10}$, and let $y_{n+1}^{(4,2)}$ denote the discrete solution when $\mu = \frac{1}{2} + i\,\frac{1}{2}\,\tan\frac{3\pi}{10}$. Define p and q by

$$p := \tan\frac{\pi}{10}\left(\sec\frac{\pi}{10}\right)^5 \tag{6.15a}$$

and

$$q := \tan\frac{3\,\pi}{10}\left(\sec\frac{3\,\pi}{10}\right)^5. \tag{6.15b}$$

Then the extrapolated solution

$$y_{n+1}^{(4,e)} := \frac{q\,y_{n+1}^{(4,1)} + p\,y_{n+1}^{(4,2)}}{p + q} \tag{6.16}$$

satisfies

$$y_{n+1}^{(4,e)} = y(t_{n+1}) + O(h^9) \tag{6.17}$$

so that $y_{n+1}^{(4,e)}$ is eighth-order-accurate.

The stability region of the above extrapolation for problem (5.1) is shown in Figure 13. Figure 14 shows reduction of error with stepsize for Problems 1 - 5 using $\mu = \frac{1}{2} + i\,\frac{1}{2}\,\tan\frac{\pi}{10}$, $\mu = \frac{1}{2} + i\,\frac{1}{2}\,\tan\frac{3\pi}{10}$, and extrapolation. Table X shows the corresponding orders of accuracy.

Operation	Corrector Iteration	Newton Iteration
Function Evaluations	4 M + 4	5 M + 4
Additions and Subtractions	4 M + 4	10 M + 4
Multiplications	4 M + 4	8 M + 4
Divisions	0	M

Table IX Computational work per step for a degree-4 Taylor series with $\mu = \frac{1}{2} \pm i\,\frac{1}{2}\tan\frac{\pi}{10}$ or $\mu = \frac{1}{2} \pm i\,\frac{1}{2}\tan\frac{3\pi}{10}$.

Expansion Coefficient	Problem: 1	2	3	4	5
$\mu = \frac{1}{2} + i\,\frac{1}{2}\tan\frac{\pi}{10}$	6.00	5.94	6.01	5.99	5.89
$\mu = \frac{1}{2} + i\,\frac{1}{2}\tan\frac{3\pi}{10}$	6.00	5.80	5.92	6.00	6.27
extrapolation	7.98	7.62	8.01	7.97	7.89

Table X Numerical order of accuracy for Problems 1 - 5 using a degree-4 Taylor series.

Extrapolation for Taylor Series of Arbitrary Degree

According to our work in the two previous sections, a degree-3 Taylor series with extrapolation provides a sixth-order method, and a degree-4 Taylor series with extrapolation provides an eighth-order method. In general, if k is odd, a degree-k Taylor series with extrapolation provides a $(k+3)$rd-order method, and if k is even, a degree-k Taylor series with extrapolation provides a $(k+4)$th-order method. The purpose of this section is to generalize these results.

Let $y_{n+1}^{(k,e)}$ denote the extrapolated solution of degree k at t_{n+1}. Let $y_{n+1}^{(k,1)}$ and $y_{n+1}^{(k,2)}$ denote the regular solution of degree k at t_{n+1} corresponding to $\mu = \mu_1$ and $\mu = \mu_2$, respectively, where μ_1 and μ_2 are defined as follows. For k odd, let

$$\mu_1 = \frac{1}{2} \tag{6.18a}$$

and

$$\mu_2 = \frac{1}{2} + i\frac{1}{2}\tan\frac{\pi}{k+1}. \tag{6.18b}$$

For k even let

$$\mu_1 = \frac{1}{2} + i\frac{1}{2}\tan\frac{\pi}{2(k+1)} \tag{6.19a}$$

and

$$\mu_2 = \frac{1}{2} + i\frac{1}{2}\tan\frac{3\pi}{2(k+1)}. \tag{6.19b}$$

The extrapolated solution for all k is then

$$y_{n+1}^{(k,e)} := \frac{q\, y_{n+1}^{(k,1)} + p\, y_{n+1}^{(k,2)}}{p + q} \tag{6.20}$$

where p and q are defined below. For all odd $k \geq 3$,

$$p = 1 \tag{6.21a}$$

and

$$q = \left(\sec\frac{\pi}{k+1}\right)^{k+1}. \tag{6.21b}$$

For all even $k \geq 4$,

$$p = \tan\frac{\pi}{2(k+1)}\left[\sec\frac{\pi}{2(k+1)}\right]^{k+1} \tag{6.22a}$$

and

$$q = \tan\frac{3\pi}{2(k+1)}\left[\sec\frac{3\pi}{2(k+1)}\right]^{k+1}. \tag{6.22b}$$

Using the above formulas, we implemented extrapolation schemes of degree five and six. Figure 15 shows the corresponding stability regions for problem (5.1). Application to Problem 1 produced the results shown in Figures 16.a,b, where the numerical orders of accuracy are 8.01 and 9.87, respectively.

Numerical Results - Variable Stepsize

The purpose of this section is to briefly introduce a variable step approach that can be implemented using an implicit Taylor series method. Here we present results for Problems 1 - 5, and in the next two sections we consider singular equations and stiff systems.

To develop a variable step scheme, one must have a method for estimating the local error and a procedure for controlling the stepsize. For an implicit series of degree three or higher, the local error can be obtained by extrapolation. For a degree-two series, the error can be obtained by integrating twice at each step – once with (3.13) and once with (3.14). The difference between the two solutions is an $O(h^3)$ error estimate. Similarly, one integrates with (2.12) and (2.5) when using a series of first degree.

The stepsize may be adjusted as follows. Let e_n denote the error at step n, and let τ be the error tolerance. Then if e_n is $O(h^\rho)$ and h_n is a successful stepsize, an estimate for h_{n+1} is

$$h_{n+1} = \xi \, h_n \left(\frac{\tau}{e_n}\right)^{\frac{1}{\rho}} \tag{7.1}$$

where ξ is an adjustable parameter less than one [28]. (See [29] for a discussion of stepsize control for long Taylor series methods.)

In what follows, we present numerical results from four variable step schemes, which we identify as follows. Scheme 1 is the degree-1 Taylor series (2.12) combined with (2.5). Scheme 2 is the degree-2 series (3.13) combined with (3.14). Schemes 3 and 4 are the degree-3 and -4 series with extrapolation, respectively. See Table XI.

Scheme	Taylor Series	Order of Accuracy	ρ
1	Degree 1	2nd	2
2	Degree 2	4th	3
3	Degree 3	6th	5
4	Degree 4	8th	7

Table XI   Variable step schemes with their orders of accuracy and ρ values.

We integrated Problems 1 - 5 on the interval [0,20]. For Schemes 2 - 4, the initial stepsize was determined from $\frac{h^k}{k!} f^{(k-1)} < \tau$, where k is the degree of the corresponding Taylor series and the total derivative $f^{(k-1)}$ was evaluated near t_0 but not at t_0. For Scheme 1, we used $\frac{h^2}{2} \lambda^2 < \tau$, where $\lambda = \frac{\partial f}{\partial y}$ [30]. Subsequent stepsizes were determined from (7.1), subject to $\frac{h_{n+1}}{h_n} \leq h_{\text{fact}}$, where $h_{\text{fact}} = 2.0$. We took ξ to be 0.9 for Schemes 2 - 4 and 0.7 for Scheme 1. Unsuccessful stepsizes h'_{n+1} were reduced using $h_{n+1} := \nu \, h'_{n+1}$, where $\nu = 0.7$. At the initial step we took $\nu = 0.1$. All parameters identified above were maintained at their stated values for all calculations.

For each problem, we varied the tolerance from 10^{-2} to 10^{-12}, and determined the maximum absolute error and number of integration steps per tolerance. The results are shown in Tables XII - XVI. The average number of repeat steps per tolerance is stated at the bottom of each table.

	Scheme:			
Tolerance	1	2	3	4
0.10E-01	0.0740	0.0437	0.0291	0.0150
0.10E-02	0.0789	0.0453	0.0328	0.0209
0.10E-03	0.0807	0.0447	0.0331	0.0212
0.10E-04	0.0814	0.0454	0.0327	0.0212
0.10E-05	0.0816	0.0454	0.0329	0.0210
0.10E-06	0.0816	0.0452	0.0327	0.0213
0.10E-07	0.0817	0.0450	0.0329	0.0208
0.10E-08	0.0817	0.0439	0.0331	0.0200
0.10E-09	0.0817	0.0355	0.0297	0.0196
0.10E-10	0.0817	0.0229	0.0231	0.0171
0.10E-11	0.1690	0.0128	0.0166	0.0147

Table XII.a Maximum error in units of the error tolerance for Problem 1.

	Scheme:			
Tolerance	1	2	3	4
0.10E-01	24	11	8	7
0.10E-02	68	18	11	9
0.10E-03	205	32	15	11
0.10E-04	642	61	21	14
0.10E-05	2023	124	31	17
0.10E-06	6391	258	46	23
0.10E-07	20204	545	70	30
0.10E-08	63886	1164	108	39
0.10E-09	202023	2497	167	53
0.10E-10	638849	5368	260	71
0.10E-11	2020214	11553	407	96

Table XII.b Number of integration steps per tolerance for Problem 1. Average number of repeat steps is 0.00 for all four schemes.

Tolerance	Scheme: 1	2	3	4
0.10E-01	0.0447	0.0179	0.0129	0.0026
0.10E-02	0.0509	0.0195	0.0330	0.0127
0.10E-03	0.0530	0.0149	0.0447	0.0220
0.10E-04	0.0536	0.0090	0.0491	0.0312
0.10E-05	0.0538	0.0047	0.0463	0.0389
0.10E-06	0.0539	0.0023	0.0391	0.0439
0.10E-07	0.0539	0.0011	0.0300	0.0453
0.10E-08	0.0539	0.0005	0.0217	0.0430
0.10E-09	0.0539	0.0003	0.0149	0.0384
0.10E-10	0.0777	0.0004	0.0100	0.0325
0.10E-11	0.2639	0.0043	0.0067	0.0267

Table XIII.a Maximum error in units of the error tolerance for Problem 2.

Tolerance	Scheme: 1	2	3	4
0.10E-01	22	10	8	7
0.10E-02	62	17	10	8
0.10E-03	189	31	13	10
0.10E-04	593	60	18	13
0.10E-05	1868	121	25	16
0.10E-06	5899	252	37	20
0.10E-07	18649	535	54	26
0.10E-08	58968	1143	82	34
0.10E-09	186466	2453	125	45
0.10E-10	589650	5275	194	60
0.10E-11	1864632	11352	303	81

Table XIII.b Number of integration steps per tolerance for Problem 2. Average number of repeat steps is 0.00 for all four schemes.

Tolerance	Scheme: 1	2	3	4
0.10E-01	0.3811	0.1431	2.7849	1.4753
0.10E-02	0.4194	0.1012	1.6676	6.0293
0.10E-03	0.5615	0.0338	0.4951	2.9164
0.10E-04	0.6472	0.0394	0.3809	0.9818
0.10E-05	0.9096	0.0187	0.0843	0.6711
0.10E-06	0.8700	0.0112	0.1057	2.0509
0.10E-07	0.9516	0.0072	0.1928	0.2164
0.10E-08	1.0210	0.0035	0.0881	0.3157
0.10E-09	1.1632	0.0019	0.0953	0.3654
0.10E-10	1.5815	0.0139	0.0205	0.2030
0.10E-11	6.7590	0.2318	0.0355	0.1470

Table XIV.a Maximum error in units of the error tolerance for Problem 3.

Tolerance	Scheme: 1	2	3	4
0.10E-01	189	48	24	18
0.10E-02	583	91	35	24
0.10E-03	1833	182	54	32
0.10E-04	5785	374	81	45
0.10E-05	18282	786	124	59
0.10E-06	57802	1676	189	78
0.10E-07	182774	3587	293	109
0.10E-08	577969	7706	457	148
0.10E-09	1827690	16580	718	200
0.10E-10	5779651	35699	1129	275
0.10E-11	18276843	76885	1784	376

Table XIV.b Number of integration steps per tolerance for Problem 3. Average number of repeat steps is 13.27, 39.55, 21.55, and 18.64, respectively.

Tolerance	Scheme: 1	2	3	4
0.10E-01	0.5808	0.0845	0.1886	0.1124
0.10E-02	0.6372	0.0447	0.0563	0.2916
0.10E-03	0.7465	0.0358	0.0960	0.1249
0.10E-04	0.7706	0.0253	0.1353	0.1802
0.10E-05	0.8511	0.0176	0.1521	0.1105
0.10E-06	0.8976	0.0132	0.1325	0.0940
0.10E-07	0.9536	0.0070	0.1009	0.0655
0.10E-08	1.0350	0.0049	0.0670	0.0680
0.10E-09	1.0712	0.0031	0.0706	0.0458
0.10E-10	1.3559	0.0064	0.0375	0.0276
0.10E-11	6.3949	0.1315	0.0426	0.0249

Table XV.a Maximum error in units of the error tolerance for Problem 4.

Tolerance	Scheme: 1	2	3	4
0.10E-01	61	15	9	8
0.10E-02	188	26	12	9
0.10E-03	587	48	16	11
0.10E-04	1851	94	22	13
0.10E-05	5845	193	31	17
0.10E-06	18476	406	45	21
0.10E-07	58421	864	68	27
0.10E-08	184736	1849	102	35
0.10E-09	584179	3973	157	46
0.10E-10	1847330	8546	244	61
0.10E-11	5841766	18398	382	81

Table XV.b Number of integration steps per tolerance for Problem 4. Average number of repeat steps is 1.82, 5.64, 2.00, and 2.45, respectively.

Scheme:

Tolerance	1	2	3	4
0.10E-01	0.8047	0.4356	0.2230	0.0720
0.10E-02	0.8404	0.3574	0.4007	0.1866
0.10E-03	0.8525	0.2637	0.4884	0.3063
0.10E-04	0.8564	0.1598	0.5048	0.4553
0.10E-05	0.8576	0.0965	0.4550	0.5675
0.10E-06	0.8580	0.0512	0.3541	0.5609
0.10E-07	0.8582	0.0293	0.2658	0.5781
0.10E-08	0.8584	0.0154	0.1848	0.5165
0.10E-09	0.9120	0.0109	0.1254	0.4395
0.10E-10	0.6662	0.0266	0.0828	0.3670
0.10E-11	12.1506	0.1926	0.0400	0.3304

Table XVI.a Maximum error in units of the error tolerance for Problem 5.

Scheme:

Tolerance	1	2	3	4
0.10E-01	66	13	8	7
0.10E-02	203	23	11	8
0.10E-03	635	41	15	10
0.10E-04	2003	82	21	13
0.10E-05	6328	169	30	16
0.10E-06	20005	355	45	21
0.10E-07	63254	757	68	28
0.10E-08	200021	1620	104	36
0.10E-09	632515	3479	161	49
0.10E-10	2000183	7484	251	65
0.10E-11	6325129	16113	393	88

Table XVI.b Number of integration steps per tolerance for Problem 5. Average number of repeat steps is 0.00, 3.36, 0.00, and 0.00, respectively.

Numerical Results - ODE's with a Singular Point

Three ODE's with a regular singularity at the origin are Bessel's equation,

$$x^2 y'' + x y' + (x^2 - k^2) y = 0 \tag{8.1}$$

Coulomb's equation,

$$x^2 y'' + \left[-L(L+1) - 2\eta x + x^2\right] y = 0 \tag{8.2}$$

and the hypergeometric equation (Gauss's equation)

$$x(1-x) y'' + \left[\gamma - (\alpha+\beta+1) x\right] y' - \alpha\beta y = 0. \tag{8.3}$$

The above equations are typical of a large class of linear, second-order equations from mathematical physics with a regular singular point. A general approach for integrating such equations has been presented by Holubec and Stauffer [31]. Haftel *et. al.* [32] presented a similar approach for coupled systems. We show here that implicit Taylor series methods can directly integrate such problems as a special case. We consider the following set of model problems.

Problem	ODE	Initial Condition	Exact Solution
6.a	(8.1) with $k = 0$	$y(0) = 1$ $y'(0) = 0$	J_0
6.b	(8.1) with $k = 1$	$y(0) = 0$ $y'(0) = 1/2$	J_1
7.	(8.2) with $L = 0$, $\eta = 1$	$y(0) = 0$ $y'(0) = e^{-\frac{\pi}{2}}\sqrt{\pi/\sinh\pi}$	Coulomb Wavefunction
8.a	(8.3) with $\alpha = 0.4$, $\beta = 1.0$, $\gamma = 0.5$	$y(0) = 1$ $y'(0) = 0.8$	Hypergeometric Function
8.b	(8.3) with $\alpha = 0.5$, $\beta = 0.5$, $\gamma = 1.5$	$y(0) = 1$ $y'(0) = 1/6$	Hypergeometric Function

We first looked at order of accuracy near the singular point. Each problem was reformulated as a system of two first order equations in the usual way. Problems 6 and 7 were integrated on [0,1], and Problem 8 on $[0, \frac{1}{2}]$. Error reduction results are plotted in Figures 17 - 19, and the corresponding orders of accuracy are summarized in Table XVII.

It is evident that a significant loss of accuracy occurred on Problems 6.b and 7. The degree-4 Taylor series lost from one to four orders of accuracy, while the degree-2 and -3 series lost from one to two orders. However, it should be noted that the orders of accuracy above are as high or higher than an explicit Taylor series of the same degree would be for a nonsingular problem. We also observe from Figures 17 - 19 that without exception the extrapolated solution for the degree-3 and -4 Taylor series is more accurate than the non-extrapolated solutions.

To look at variable step performance, we used Schemes 1 - 4 to solve Problems 6.a,b on the interval [0,20]. Each scheme was used as described in Section 7, with appropriate modifications for a system. The results shown in Tables XVIII - IXX are indeed comparable to those in Tables XII - XVI for the nonsingular Problems 1 - 5.

	Problem:				
	6.a	6.b	7	8.a	8.b
Taylor Series					
Degree-1					
$\mu = \frac{1}{2}$	2.00	1.89	1.85	2.01	1.92
Degree-2					
$\mu = \frac{1}{2} + i\frac{\sqrt{3}}{6}$	3.93	2.00	3.02	3.82	4.07
Degree-3					
$\mu = \frac{1}{2}$	3.99	3.89	3.82	4.01	3.88
$\mu = \frac{1}{2} + i\frac{1}{2}$	3.99	3.89	3.81	3.84	3.77
extrapolation	5.83	4.47	4.21	5.57	5.77
Degree-4					
$\mu = \frac{1}{2} + i\frac{1}{2}\tan\frac{\pi}{10}$	5.92	4.01	4.99	5.84	5.75
$\mu = \frac{1}{2} + i\frac{1}{2}\tan\frac{3\pi}{10}$	5.92	4.10	5.02	5.70	5.62
extrapolation	5.83	3.94	4.83	7.20	7.48

Table XVII Order of accuracy near a regular singular point.

Scheme:

Tolerance	1	2	3	4
0.10E-01	1.0965	1.7756	0.4928	1.1900
0.10E-02	1.0755	0.5731	0.4334	1.0079
0.10E-03	1.0736	0.2519	0.2957	0.4966
0.10E-04	1.0733	0.1157	0.2076	0.3070
0.10E-05	1.0732	0.0536	0.1335	0.2350
0.10E-06	1.0732	0.0249	0.0849	0.1643
0.10E-07	1.0732	0.0116	0.0543	0.1179
0.10E-08	1.0733	0.0054	0.0340	0.0878
0.10E-09	1.0744	0.0024	0.0216	0.0624
0.10E-10	1.1015	0.0012	0.0130	0.0622
0.10E-11	1.3933	0.0212	0.0106	0.0892

Table XVIII.a Maximum error in units of the error tolerance for Problem 6.a.

Scheme:

Tolerance	1	2	3	4
0.10E-01	114	24	15	13
0.10E-02	332	51	23	18
0.10E-03	1021	107	34	22
0.10E-04	3198	226	52	28
0.10E-05	10083	481	81	37
0.10E-06	31854	1032	125	49
0.10E-07	100701	2217	196	66
0.10E-08	318415	4769	308	89
0.10E-09	1006888	10269	484	120
0.10E-10	3184029	22115	764	164
0.10E-11	10068755	47639	1206	225

Table XVIII.b Number of integration steps per tolerance for Problem 6.a. Average number of repeat steps is 0.00, 0.09, 0.64, and 0.45, respectively.

Tolerance	Scheme: 1	2	3	4
0.10E-01	1.1825	2.0417	0.5799	3.3158
0.10E-02	1.1569	0.6318	0.4310	0.8488
0.10E-03	1.1535	0.2763	0.3510	0.5983
0.10E-04	1.1521	0.1262	0.2365	0.3736
0.10E-05	1.1511	0.1003	0.1515	0.2587
0.10E-06	1.1505	0.1007	0.0958	0.1845
0.10E-07	1.1502	0.0993	0.0604	0.1307
0.10E-08	1.1501	0.0941	0.0378	0.0940
0.10E-09	1.1492	0.0832	0.0237	0.0736
0.10E-10	1.1454	0.0720	0.0172	0.2112
0.10E-11	1.3087	0.0774	0.0201	0.5614

Table IXX.a Maximum error in units of the error tolerance for Problem 6.b.

Tolerance	Scheme: 1	2	3	4
0.10E-01	113	24	18	19
0.10E-02	326	50	25	23
0.10E-03	1000	106	37	27
0.10E-04	3131	224	55	34
0.10E-05	9869	477	83	42
0.10E-06	31177	1022	127	54
0.10E-07	98557	2194	197	71
0.10E-08	311633	4718	308	93
0.10E-09	985438	10152	484	125
0.10E-10	3116197	21855	761	169
0.10E-11	9854247	47063	1200	229

Table IXX.b Number of integration steps per tolerance for Problem 6.b. Average number of repeat steps is 0.00, 0.09, 0.09, and 0.00, respectively.

Numerical Results - Stiff Equations

In this section we briefly consider stiff equations. For a set of model problems we use Problems 9 - 13 below.

Problem 9: (Enright and Pryce [33], Problem A3)

$$\begin{aligned} y_1' &= -10^4\, y_1 + 100\, y_2 - 10\, y_3 + y_4 \\ y_2' &= -10^3\, y_2 + 10\, y_3 - 10\, y_4 \\ y_3' &= -y_3 + 10\, y_4 \\ y_4' &= -0.1\, y_4 \end{aligned}$$

$$y_1(0) = 1, \qquad y_2(0) = 1, \qquad y_3(0) = 1, \qquad y_4(0) = 1, \qquad t_{end} = 20$$

Problem 10: ([33], Problem B1)

$$\begin{aligned} y_1' &= -y_1 + y_2 \\ y_2' &= -100\, y_1 - y_2 \\ y_3' &= -100\, y_3 + y_4 \\ y_4' &= -10^4\, y_3 - 100\, y_4 \end{aligned}$$

$$y_1(0) = 1, \qquad y_2(0) = 0, \qquad y_3(0) = 1, \qquad y_4(0) = 0, \qquad t_{end} = 20$$

Problem 11: ([33], Problem D4)

$$\begin{aligned} y_1' &= -0.013\, y_1 - 1000\, y_1\, y_3 \\ y_2' &= -2500\, y_2\, y_3 \\ y_3' &= -0.013\, y_1 - 1000\, y_1\, y_3 - 2500\, y_2\, y_3 \end{aligned}$$

$$y_1(0) = 1, \qquad y_2(0) = 1, \qquad y_3(0) = 0, \qquad t_{end} = 50$$

Problem 12: (Robertson [34])

$$y_1' = -0.04\,y_1 + 10^4\,y_2\,y_3$$

$$y_2' = 0.04\,y_1 - 10^4\,y_2\,y_3 - 3\cdot 10^7\,y_2^2$$

$$y_3' = 3\cdot 10^7\,y_2^2$$

$$y_1(0)=1, \qquad y_2(0)=0, \qquad y_3(0)=0, \qquad t_{end}=40$$

Problem 13: ([33], Problem F3)

$$y_1' = -10^7\,y_2\,y_1 + 10\,y_3$$

$$y_2' = -10^7\,y_2\,y_1 - 10^7\,y_2\,y_5 + 10\,y_3 + 10\,y_4$$

$$y_3' = 10^7\,y_2\,y_1 - 1.001\cdot 10^4\,y_3 + 10^{-3}\,y_4$$

$$y_4' = 10^4\,y_3 - 10.001\,y_4 + 10^7\,y_2\,y_5$$

$$y_5' = 10\,y_4 - 10^7\,y_2\,y_5$$

$$y_1(0)=4\cdot 10^{-6}, \qquad y_2(0)=1\cdot 10^{-6}, \qquad y_3(0)=0, \qquad y_4(0)=0, \qquad y_5(0)=0$$

$$t_{end}=100$$

We integrated each system using Schemes 1 - 4, along with a trapezoidal extrapolation scheme which we now introduce.

Let y_n^T denote the trapezoidal solution (2.15), and let $y_n^{(2)}$ denote the degree-2 Taylor series solution (3.14) with $\mu = \frac{1}{2}$. One can show that the extrapolated solution

$$y_{n+1}^e := \frac{2\,y_{n+1}^{(2)} + y_{n+1}^T}{3} \tag{9.7}$$

is A-stable and fourth-order-accurate with truncation error

$$y(t_{n+1}) \; - \; y^e_{n+1} \; = \; - \, \frac{h^5}{2880} \left[f''''_n \; + \; 5 \, \frac{\partial f_n}{\partial y} \, f'''_n \; + \; 20 \, \big(\frac{\partial^2 f_n}{\partial t \partial y} \; + \; \frac{\partial^2 f_n}{\partial y^2} \, f_n \big) \, f''_n \right]. \qquad (9.8)$$

A variable stepsize for (9.7) can be obtained using (7.1) together with the $O(h^3)$ error estimate $e_n = |y^e_{n+1} - y^{(2)}_{n+1}|$. The above extrapolation with variable step implementation will be called Scheme 2T.

In integrating Problems 9 - 13, the parameters ξ, h_{fact}, and ν, introduced in Section 7, were assigned default values of 0.9, 2.0, and 0.7, respectively, except for Scheme 1 where ξ was set to 0.7. Any deviation from these values is noted at the bottom of Tables XX - XXIV. The local error estimate e_n was taken to be the largest absolute error in any solution component. The initial stepsize was determined as in Section 7 (with appropriate modifications for a system).

Tables XX - XXI demonstrate some degradation in the ability of Schemes 1 - 4 to meet the error tolerance. Whether this holds in general for stiff problems requires further investigation.

One also observes that the eighth-order-accurate Scheme 4 frequently required more steps than some of the lower order schemes. This contrasts with the nonstiff results presented earlier, and illustrates the well known need for stiff solvers to be able to vary their order.

	Scheme:				
Tolerance	1	2	2 T	3	4
0.10E-01	0.1512	0.0485	0.0096	0.0326	0.3952
0.10E-02	0.2270	0.0628	0.0129	0.0332	1.0237
0.10E-03	0.3221	0.1356	0.0164	0.0339	2.1679
0.10E-04	0.3287	0.1016	0.0229	0.0393	2.8883
0.10E-05	0.3292	0.0450	0.0155	0.0488	6.2514
0.10E-06	0.3293	0.0453	0.0100	0.0695	4.1981
0.10E-07	0.3293	0.0455	0.0095	0.4929	6.7522
0.10E-08	0.3295	0.0443	0.0095	0.5759	5.6286
0.10E-09	0.3265	0.0327	0.0086	1.9309	6.1883
0.10E-10	0.4206	0.0176	0.0061	5.1021	9.4324
0.10E-11	1.4309	0.1217	0.3659	5.7487	5.8660

Table XX.a Maximum error in units of the error tolerance for Problem 9.

	Scheme:				
	1	2	2 T	3	4
Tolerance					
0.10E-01	121	34	34	24	31
0.10E-02	369	60	60	32	34
0.10E-03	1157	116	116	44	41
0.10E-04	3654	236	236	65	53
0.10E-05	11551	496	496	96	72
0.10E-06	36525	1055	1055	145	105
0.10E-07	115498	2259	2259	224	163
0.10E-08	365234	4851	4851	349	249
0.10E-09	1154967	10438	10438	547	406
0.10E-10	3652325	22473	22473	883	662
0.10E-11	11549662	48402	48402	1450	1119

Table XX.b Number of integration steps per error tolerance for Problem 9. Average number of repeat steps is 0.18, 0.91, 1.18, 5.82, and 13.00, respectively. Changes to default values: Scheme 3, $\nu = 0.5$; Scheme 4, $h_{\text{fact}} = 1.5$, $\nu = 0.5$.

	Scheme:				
	1	2	2 T	3	4
Tolerance					
0.10E-01	1.5593	2.8866	0.4222	0.7640	7.1984
0.10E-02	2.0085	3.0205	0.6115	0.8367	3.7537
0.10E-03	2.0902	2.1121	0.6816	0.5848	3.2502
0.10E-04	2.1074	3.2174	0.4245	0.9580	11.8994
0.10E-05	2.1121	3.3088	0.7441	0.6915	4.3284
0.10E-06	2.1134	2.2518	0.7997	0.5903	3.3849
0.10E-07	2.1141	2.8611	0.4129	0.8654	2.0479
0.10E-08	2.1142	0.9528	0.2677	0.3111	2.3132
0.10E-09	2.1166	0.4421	0.1545	0.2352	0.4552
0.10E-10	2.1143	0.2346	0.1879	0.2052	0.2391
0.10E-11	17.8417	0.4707	2.7374	0.1712	0.1882

Table XXI.a Maximum error in units of the error tolerance for Problem 10.

Tolerance	Scheme: 1	2	2 T	3	4
0.10E-01	712	135	142	73	44
0.10E-02	2219	299	304	118	70
0.10E-03	6992	642	648	192	105
0.10E-04	22082	1380	1389	307	147
0.10E-05	69805	2969	2978	486	211
0.10E-06	220720	6395	6397	766	297
0.10E-07	697952	13771	13775	1208	413
0.10E-08	2207094	29655	29656	1905	571
0.10E-09	6979416	63864	63864	3008	792
0.10E-10	22070843	137568	137569	4757	1092
0.10E-11	69794029	296360	296361	7528	1512

Table XXI.b Number of integration steps per error tolerance for Problem 10. Average number of repeat steps is 19.45, 26.64, 26.73, 19.18, and 10.00, respectively. Changes to default values: Scheme 1, $\nu = 0.5$; Scheme 2, $\xi = 0.8$; Scheme 2T, $\xi = 0.8$; Scheme 3, $\xi = 0.8$; Scheme 4, $\xi = 0.8$, $\nu = 0.5$.

Tolerance	Scheme: 1	2	2 T	3	4
0.10E-01	23	13	13	15	40
0.10E-02	31	15	15	16	44
0.10E-03	56	17	17	17	46
0.10E-04	135	21	21	18	44
0.10E-05	387	29	29	19	46
0.10E-06	1187	46	46	22	48
0.10E-07	3720	83	83	26	51
0.10E-08	11734	164	164	32	54
0.10E-09	37081	337	337	43	77
0.10E-10	117237	710	710	60	117
0.10E-11	370738	1515	1515	89	189

Table XXII Number of integration steps per error tolerance for Problem 11. Average number of repeat steps is 0.00, 1.45, 1.55, 0.09, and 10.36, respectively. Changes to default values: Scheme 3, $\nu = 0.5$; Scheme 4, $\xi = 0.8$, $h_{\text{fact}} = 1.5$, $\nu = 0.5$.

Tolerance	Scheme: 1	2	2 T	3	4
0.10E-01	29	15	26	41	85
0.10E-02	48	91	22	43	79
0.10E-03	109	715	25	45	90
0.10E-04	303	41	41	47	73
0.10E-05	920	75	77	47	72
0.10E-06	2874	153	154	49	77
0.10E-07	9054	319	321	60	74
0.10E-08	28599	676	679	78	78
0.10E-09	90406	1448	1450	112	84
0.10E-10	285857	3108	3111	164	115
0.10E-11	903936	6686	6688	249	168

Table XXIII Number of integration steps per error tolerance for Problem 12. Average number of repeat steps is 0.00, 3.91, 2.82, 5.55, and 28.18, respectively. Changes to default values: Scheme 2, $\nu = 0.5$; Scheme 2T, $\nu = 0.5$; Scheme 3, $\xi = 0.8$, $h_{\text{fact}} = 1.5$, $\nu = 0.5$; Scheme 4, $\xi = 0.8$, $h_{\text{fact}} = 1.5$, $\nu = 0.5$.

Tolerance	Scheme: 1	2	2 T	3	4
0.10E-01	25	11	11	14	32
0.10E-02	26	13	13	15	30
0.10E-03	28	15	15	17	31
0.10E-04	30	16	16	18	36
0.10E-05	32	18	18	19	34
0.10E-06	41	21	20	20	36
0.10E-07	77	28	27	23	37
0.10E-08	192	43	43	29	39
0.10E-09	561	78	77	38	43
0.10E-10	1729	151	150	53	50
0.10E-11	5425	308	307	78	61

Table XXIV Number of integration steps per error tolerance for Problem 13. Average number of repeat steps is 0.00, 0.00, 0.00, 0.00, and 4.09, respectively. Changes to default values: Scheme 4, $\xi = 0.8$, $h_{\text{fact}} = 1.5$, $\nu = 0.5$.

Discussion and Conclusion

In this paper we have presented a new class of implicit Taylor series methods for solving ODE initial value problems. Based on the results presented herein, we conclude that the main advantages of implicit series methods are (i) ability to achieve high accuracy while maintaining stability, (ii) robustness, (iii) simplicity, and (iv) versatility (ability to solve a wide range of problems).

However, implicit series methods suffer the disadvantage of being computationally intensive. Table XXV summarizes the median number of Newton iterations per step for the results presented in the last three sections. The Newton convergence criteria for these results was that successive solution iterates differ by less than 10^{-14}.

It is seen that a minimum of four Newton iterations are required per step – two iterations for each independent solution calculated. This means that, for a system of equations, at least two L-U decompositions must be performed at each step. Consequently, an implicit series method must be able to solve a given problem in relatively fewer steps to be competitive with other methods. For most nonstiff problems, this implies the need for a series with high order accuracy. For stiff problems, this implies the need to vary the order of accuracy during the calculation.

We conclude with the following remarks. First, for nonstiff problems, corrector iteration is an attractive alternative to Newton iteration. It is easier to implement, requires less derivative information, and for small error tolerances is often more computationally efficient. It works especially well for small, uniform stepsizes. Second, for problems without a singular point, Scheme 2T is preferred over Scheme 2. Although both schemes employ a degree-two Taylor series, use the same local error estimate (to $O(h^5)$), and generally require the same number of marching steps, Scheme 2T can be programmed in real arithmetic and is significantly faster as a result. Third, due to the length of this paper, we have not made any direct comparisons with other methods. Comparing the efficiency and reliability of integration methods has practically become a specialty in itself, and requires considerable care and discussion. The intent here is to present enough results to give some idea of performance on a range of problems. The next step toward a full comparison with other methods is to extend implicit series methods to become a variable order approach. This is proposed as a future research topic. Fourth, and lastly, implicit Taylor series methods offer a unique combination of high accuracy, stability, robustness, and versatility. The author is not aware of another existing method that can, without modification, solve both regular ODE's and stiff systems, together with linear and nonlinear ODE's with a singular point – all with an arbitrarily high order of accuracy. With computer speed and memory steadily increasing, algorithm features such as robustness, versatility, and ease of use are becoming increasingly important. For this reason, implicit Taylor series methods merit consideration as a standard integration tool for solving ordinary differential equations.

Scheme	1	2	3	4	5	6a	6b
	Problem:						
1	4.00	5.00	4.00	5.00	4.92	4.00	4.00
2	4.00	5.97	4.12	5.73	5.73	4.00	4.00
3	4.00	7.72	4.33	7.94	6.90	4.00	4.00
4	4.00	7.84	4.81	8.56	7.52	4.00	4.00

Scheme	9	10	11	12	13
1	4.00	4.00	5.95	6.00	5.56
2	4.00	4.02	6.41	7.01	5.43
2T	4.00	4.02	5.82	6.00	5.35
3	4.02	4.15	9.78	13.65	6.35
4	4.08	4.18	17.08	26.57	10.56

Table XXV Median number of Newton iterations per timestep.

Appendix

Let $y_{n+1} := y_{n+1}^{(k)}$ be the solution of

$$y_{n+1} = y_n + h\, f(t_{n+1}, y_{n+1}) - \frac{h^2}{2!}\, f'(t_{n+1}, y_{n+1}) + \frac{h^3}{3!}\, f''(t_{n+1}, y_{n+1})$$

$$- \ldots + \ldots + (-1)^{k-1}\, \frac{h^k}{k!}\, f^{(k-1)}(t_{n+1}, y_{n+1}). \tag{A.1}$$

Then for all $k \geq 2$,

$$e_{n+1}^{(k)} := y(t_{n+1}) - y_{n+1}^{(k)} =$$

$$(-1)^k \left\{ \frac{h^{k+1}}{(k+1)!}\, f_n^{(k)} + \frac{h^{k+2}}{(k+2)!} \left[(k+1)\, f_n^{(k+1)} + (k+2)\, \frac{\partial f_n}{\partial y}\, f_n^{(k)} \right] \right.$$

$$+ \frac{h^{k+3}}{(k+3)!} \left[\frac{(k+1)(k+2)}{2}\, f_n^{(k+2)} + (k+1)(k+3)\, \frac{\partial f_n}{\partial y}\, f_n^{(k+1)} \right.$$

$$\left. \left. + \frac{(k+2)(k+3)}{2}\, \frac{\partial f_n'}{\partial y}\, f_n^{(k)}) \right] \right\} + O(h^{k+4}). \tag{A.2}$$

Proof:

From equation (A.1), one can expand the solution $y_{n+1}^{(k+1)}$ in a series about the solution $y_{n+1}^{(k)}$ to obtain

$$y_{n+1}^{(k+1)} = y_n + h \left[f(t_{n+1}, y_{n+1}^{(k)}) + \left(y_{n+1}^{(k+1)} - y_{n+1}^{(k)} \right) \frac{\partial f}{\partial y}(t_{n+1}, y_{n+1}^{(k)}) \right.$$

$$\left. + \frac{1}{2} \left(y_{n+1}^{(k+1)} - y_{n+1}^{(k)} \right)^2 \frac{\partial^2 f}{\partial y^2}(t_{n+1}, y_{n+1}^{(k)}) + \ldots \right] - \frac{h^2}{2!} \left[f'(t_{n+1}, y_{n+1}^{(k)}) \right.$$

$$\left. + \left(y_{n+1}^{(k+1)} - y_{n+1}^{(k)} \right) \frac{\partial f'}{\partial y}(t_{n+1}, y_{n+1}^{(k)}) + \frac{1}{2} \left(y_{n+1}^{(k+1)} - y_{n+1}^{(k)} \right)^2 \frac{\partial^2 f'}{\partial y^2}(t_{n+1}, y_{n+1}^{(k)}) + \ldots \right]$$

$$+ \ldots - \ldots + (-1)^k\, \frac{h^{k+1}}{(k+1)!} \left[f^{(k)}(t_{n+1}, y_{n+1}^{(k)}) + \left(y_{n+1}^{(k+1)} - y_{n+1}^{(k)} \right) \frac{\partial f^{(k)}}{\partial y}(t_{n+1}, y_{n+1}^{(k)}) \right.$$

$$\left. + \frac{1}{2} \left(y_{n+1}^{(k+1)} - y_{n+1}^{(k)} \right)^2 \frac{\partial^2 f^{(k)}}{\partial y^2}(t_{n+1}, y_{n+1}^{(k)}) + \ldots \right] \tag{A.3}$$

from which one gets

$$
\begin{aligned}
y_{n+1}^{(k+1)} \;=\; & y_n \;+\; h\, f(t_{n+1}, y_{n+1}^{(k)}) \;-\; \frac{h^2}{2!}\, f'(t_{n+1}, y_{n+1}^{(k)}) \\
& + \;\ldots\; - \;\ldots\; + \;(-1)^k\, \frac{h^{k+1}}{(k+1)!}\, f^{(k)}(t_{n+1}, y_{n+1}^{(k)}) \\
& + \left(y_{n+1}^{(k+1)} \;-\; y_{n+1}^{(k)}\right) \left[h\, \frac{\partial f}{\partial y}(t_{n+1}, y_{n+1}^{(k)}) \;-\; \frac{h^2}{2!}\, \frac{\partial f'}{\partial y}(t_{n+1}, y_{n+1}^{(k)}) \right. \\
& \left. + \;\ldots\; - \;\ldots\; + \;(-1)^k\, \frac{h^{k+1}}{(k+1)!}\, \frac{\partial f^{(k)}}{\partial y}(t_{n+1}, y_{n+1}^{(k)})\right] \\
& + \frac{1}{2} \left(y_{n+1}^{(k+1)} \;-\; y_{n+1}^{(k)}\right)^2 \left[h\, \frac{\partial^2 f}{\partial y^2}(t_{n+1}, y_{n+1}^{(k)}) \;-\; \frac{h^2}{2!}\, \frac{\partial^2 f'}{\partial y^2}(t_{n+1}, y_{n+1}^{(k)}) \right. \\
& \left. + \;\ldots\; - \;\ldots\; + \;(-1)^k\, \frac{h^{k+1}}{(k+1)!}\, \frac{\partial^2 f^{(k)}}{\partial y^2}(t_{n+1}, y_{n+1}^{(k)})\right] \\
& + \;\ldots
\end{aligned}
\tag{A.4}
$$

Now

$$
\begin{aligned}
& y_n \;+\; h\, f(t_{n+1}, y_{n+1}^{(k)}) \;-\; \frac{h^2}{2!}\, f'(t_{n+1}, y_{n+1}^{(k)}) \\
& + \;\ldots\; - \;\ldots\; + \;(-1)^{k-1}\, \frac{h^k}{k!}\, f^{(k-1)}(t_{n+1}, y_{n+1}^{(k)}) \;=\; y_{n+1}^{(k)}
\end{aligned}
\tag{A.5}
$$

from equation (A.1). Therefore (A.4) becomes

$$
\begin{aligned}
y_{n+1}^{(k+1)} \;-\; y_{n+1}^{(k)} \;=\; & (-1)^k\, \frac{h^{k+1}}{(k+1)!}\, f^{(k)}(t_{n+1}, y_{n+1}^{(k)}) \\
& + \left(y_{n+1}^{(k+1)} \;-\; y_{n+1}^{(k)}\right) \left[h\, \frac{\partial f}{\partial y}(t_{n+1}, y_{n+1}^{(k)}) \;-\; \frac{h^2}{2!}\, \frac{\partial f'}{\partial y}(t_{n+1}, y_{n+1}^{(k)}) \right. \\
& \left. + \;\ldots\; - \;\ldots\; + \;(-1)^k\, \frac{h^{k+1}}{(k+1)!}\, \frac{\partial f^{(k)}}{\partial y}(t_{n+1}, y_{n+1}^{(k)})\right] \\
& + \frac{1}{2} \left(y_{n+1}^{(k+1)} \;-\; y_{n+1}^{(k)}\right)^2 \left[h\, \frac{\partial^2 f}{\partial y^2}(t_{n+1}, y_{n+1}^{(k)}) \;-\; \frac{h^2}{2!}\, \frac{\partial^2 f'}{\partial y^2}(t_{n+1}, y_{n+1}^{(k)}) \right. \\
& \left. + \;\ldots\; - \;\ldots\; + \;(-1)^k\, \frac{h^{k+1}}{(k+1)!}\, \frac{\partial^2 f^{(k)}}{\partial y^2}(t_{n+1}, y_{n+1}^{(k)})\right] \\
& + \;\ldots
\end{aligned}
\tag{A.6}
$$

It follows from (A.6) that $y_{n+1}^{(k+1)} \;-\; y_{n+1}^{(k)}$ is $O(h^{k+1})$. Retaining terms through $O(h^{k+3})$, one gets

$$y_{n+1}^{(k+1)} - y_{n+1}^{(k)} = (-1)^k \frac{h^{k+1}}{(k+1)!} f^{(k)}(t_{n+1}, y_{n+1}^{(k)})$$

$$+ \left(y_{n+1}^{(k+1)} - y_{n+1}^{(k)}\right)\left[h \frac{\partial f}{\partial y}(t_{n+1}, y_{n+1}^{(k)}) - \frac{h^2}{2}\frac{\partial f'}{\partial y}(t_{n+1}, y_{n+1}^{(k)}) + O(h^3)\right] \tag{A.7}$$

so that

$$y_{n+1}^{(k+1)} - y_{n+1}^{(k)} = (-1)^k \frac{h^{k+1}}{(k+1)!} f^{(k)}(t_{n+1}, y_{n+1}^{(k)}) \Big/$$

$$\left[1 - h \frac{\partial f}{\partial y}(t_{n+1}, y_{n+1}^{(k)}) + \frac{h^2}{2}\frac{\partial f'}{\partial y}(t_{n+1}, y_{n+1}^{(k)}) + O(h^3)\right]. \tag{A.8}$$

For sufficiently small h, one then obtains

$$y_{n+1}^{(k+1)} - y_{n+1}^{(k)} = (-1)^k \frac{h^{k+1}}{(k+1)!} f^{(k)}(t_{n+1}, y_{n+1}^{(k)}) \left\{1 + h \frac{\partial f}{\partial y}(t_{n+1}, y_{n+1}^{(k)})\right.$$

$$\left. + h^2 \left[\frac{\partial f}{\partial y}(t_{n+1}, y_{n+1}^{(k)})^2 - \frac{1}{2}\frac{\partial f'}{\partial y}(t_{n+1}, y_{n+1}^{(k)})\right]\right\} + O(h^{k+4}). \tag{A.9}$$

Now each term on the right hand side of (A.9) can be expanded in a series about (t_n, y_n), so that

$$y_{n+1}^{(k+1)} - y_{n+1}^{(k)} = (-1)^k \frac{h^{k+1}}{(k+1)!}\left[f_n^{(k)} + h \frac{\partial f_n^{(k)}}{\partial t} + \left(y_{n+1}^{(k)} - y_n\right)\frac{\partial f_n^{(k)}}{\partial y}\right.$$

$$\left. + \frac{h^2}{2}\frac{\partial^2 f_n^{(k)}}{\partial t^2} + h\left(y_{n+1}^{(k)} - y_n\right)\frac{\partial^2 f_n^{(k)}}{\partial t \partial y} + \frac{1}{2}\left(y_{n+1}^{(k)} - y_n\right)^2 \frac{\partial^2 f_n^{(k)}}{\partial y^2} + O(h^3)\right]\left[1 + h \frac{\partial f_n}{\partial y}\right.$$

$$\left. + h^2 \frac{\partial^2 f_n}{\partial t \partial y} + h\left(y_{n+1}^{(k)} - y_n\right)\frac{\partial^2 f_n}{\partial y^2} + h^2\left[\left(\frac{\partial f_n}{\partial y}\right)^2 - \frac{1}{2}\frac{\partial f_n'}{\partial y}\right] + O(h^3)\right]. \tag{A.10}$$

For all $k \geq 2$, equation (3.8) shows that

$$y_{n+1}^{(k)} - y_n = h f_n + \frac{h^2}{2} f_n' + O(h^3). \tag{A.11}$$

Substituting (A.11) into (A.10) and simplifying, one finally obtains

$$y_{n+1}^{(k+1)} - y_{n+1}^{(k)} = (-1)^k \frac{h^{k+1}}{(k+1)!}\left[f_n^{(k)} + h\left(f_n^{(k+1)} + \frac{\partial f_n}{\partial y} f_n^{(k)}\right)\right.$$

$$\left. + \frac{h^2}{2}\left(f_n^{(k+2)} + 2\frac{\partial f_n}{\partial y} f_n^{(k+1)} + \frac{\partial f_n'}{\partial y} f_n^{(k)}\right)\right]. \tag{A.12}$$

Since

$$y_{n+1}^{(k+1)} - y_{n+1}^{(k)} = y(t_{n+1}) - y_{n+1}^{(k)} - \left(y(t_{n+1}) - y_{n+1}^{(k+1)}\right) = e_{n+1}^{(k)} - e_{n+1}^{(k+1)} \quad \text{(A.13)}$$

one obtains from (A.12)

$$e_{n+1}^{(k+1)} - e_{n+1}^{(k)} = (-1)^{k+1} \frac{h^{k+1}}{(k+1)!} \left[f_n^{(k)} + h \left(f_n^{(k+1)} + \frac{\partial f_n}{\partial y} f_n^{(k)} \right) + \frac{h^2}{2} \left(f_n^{(k+2)} + 2 \frac{\partial f_n}{\partial y} f_n^{(k+1)} + \frac{\partial f_n'}{\partial y} f_n^{(k)} \right) \right]. \quad \text{(A.14)}$$

Since n and h are both fixed, (A.14) is a linear difference equation on k. One can verify by direct substitution that the solution to the difference equation is given by (A.2), plus an arbitrary constant which may be taken to be zero. Therefore (A.2) is valid for all $k \geq 2$.

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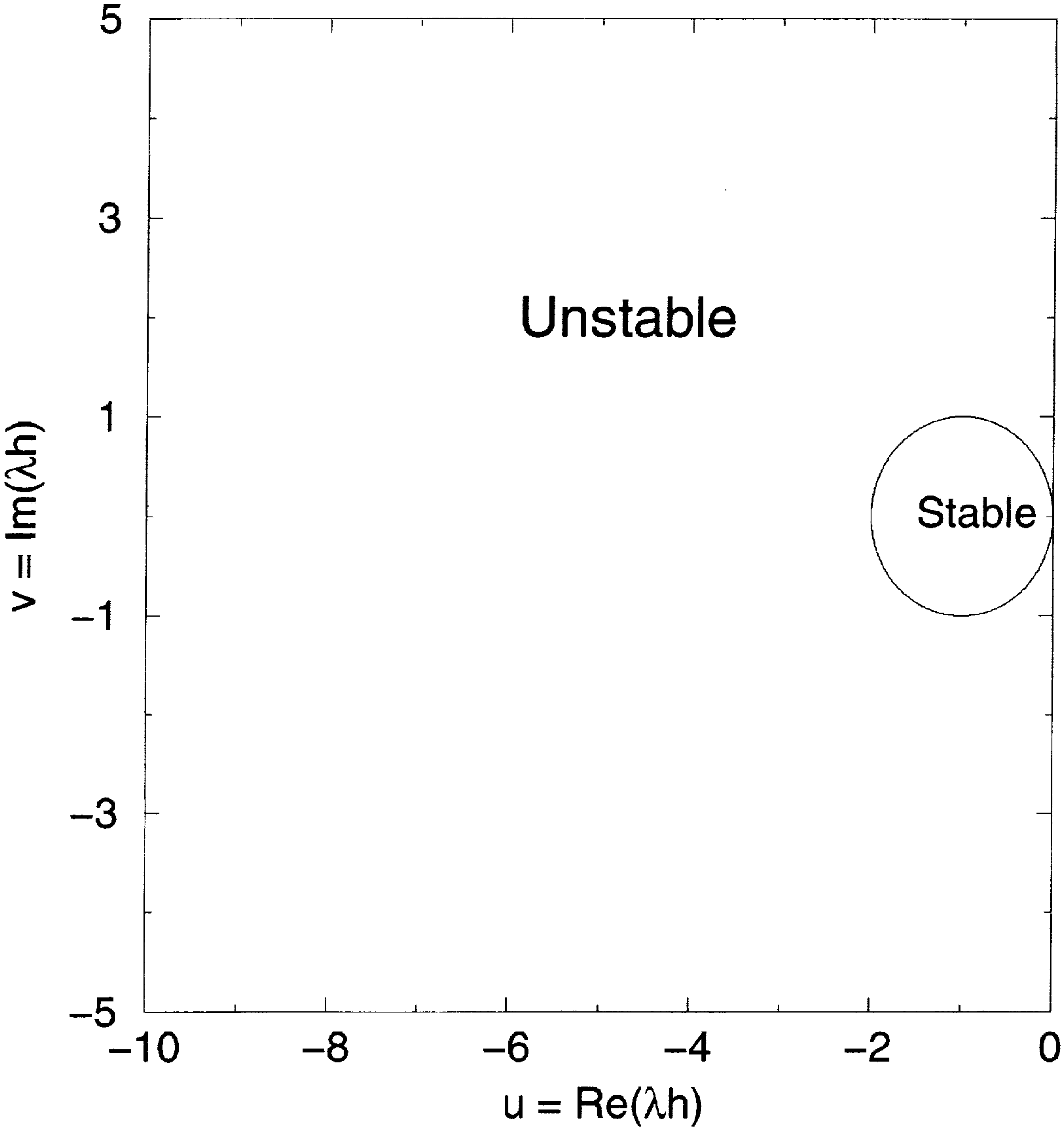

Figure 1.a Stability region for Euler's method.

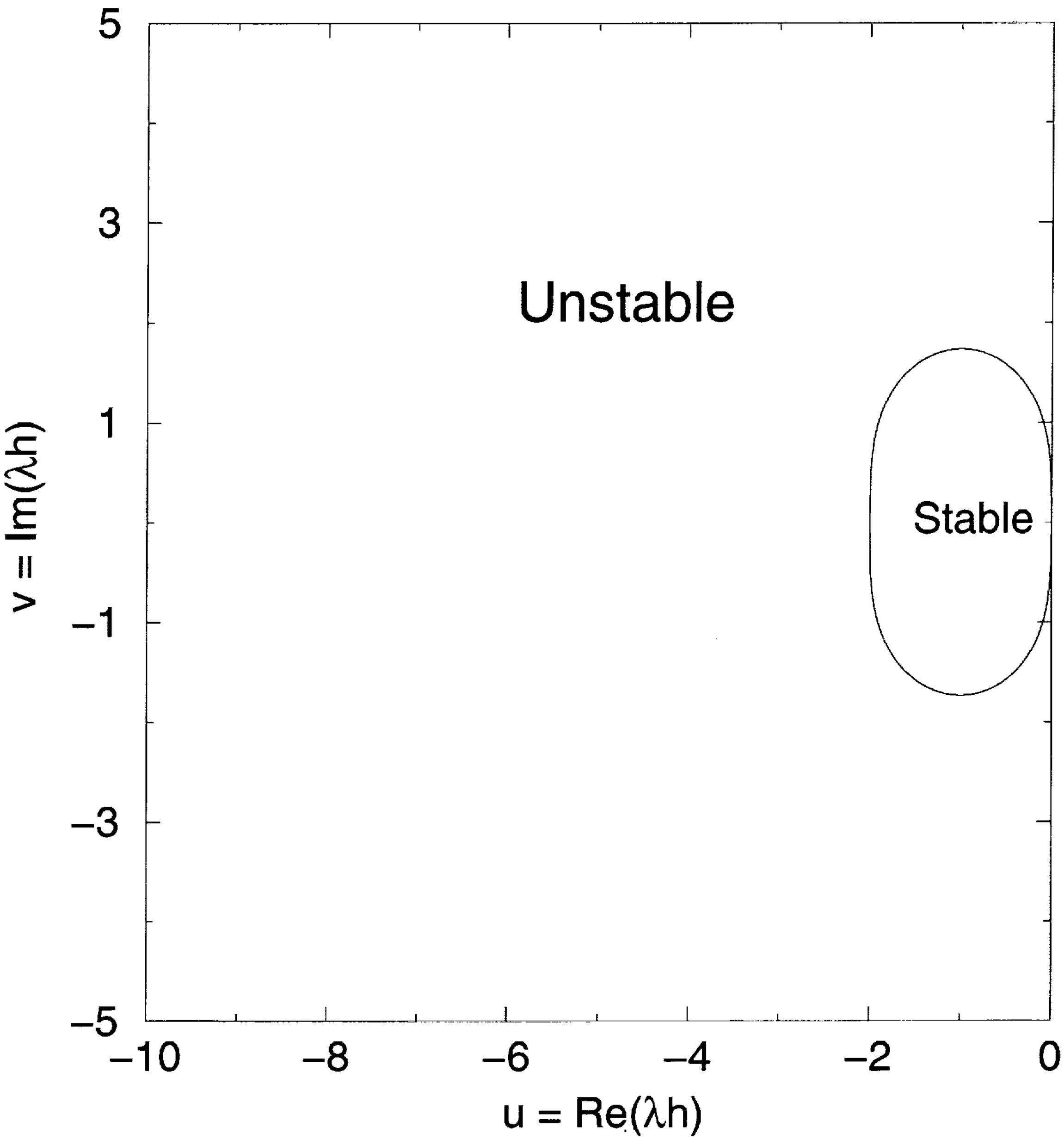

Figure 1.b Stability region for a degree-2 explicit Taylor series.

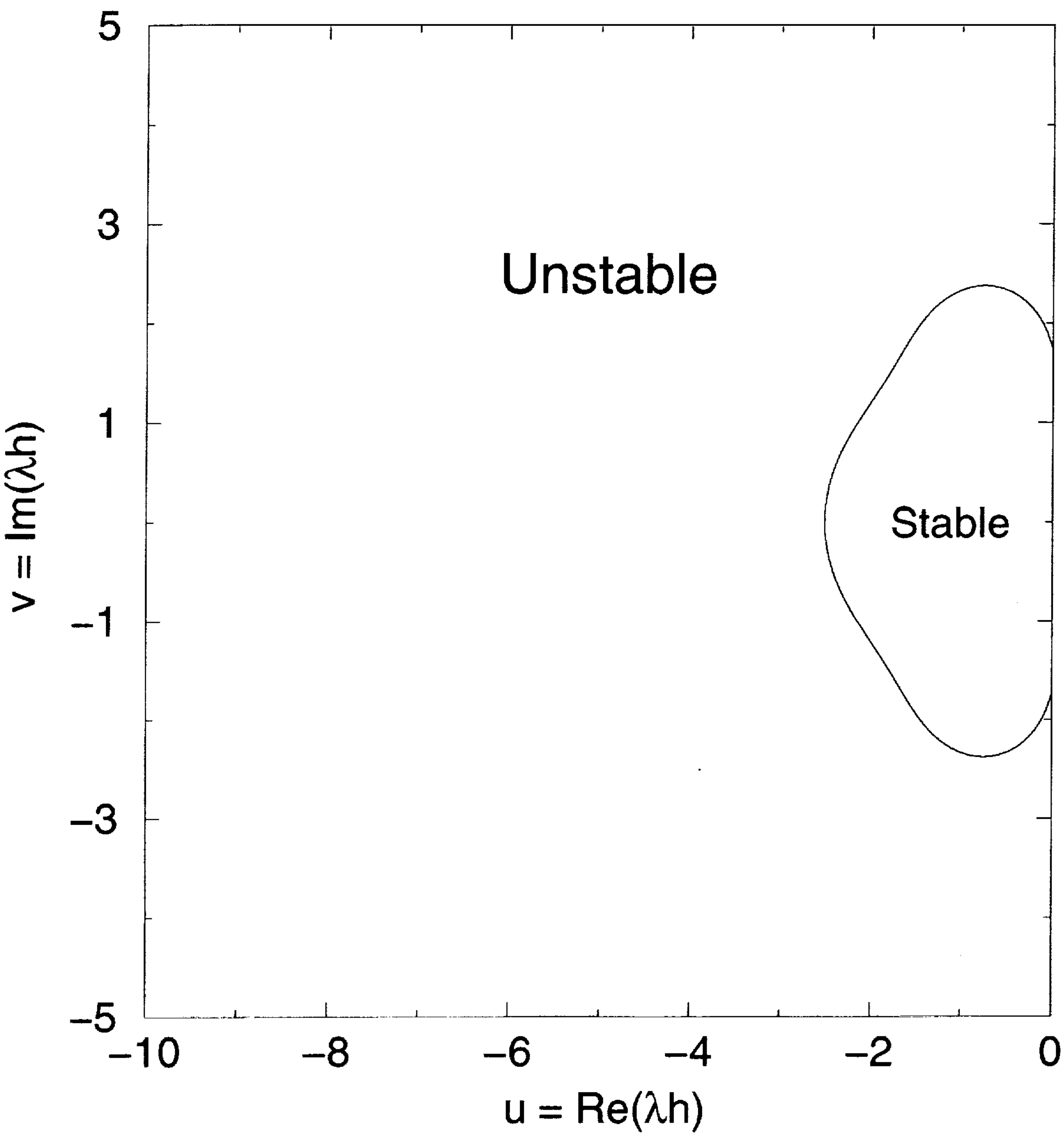

Figure 2 Stability region for a degree-3 explicit Taylor series.

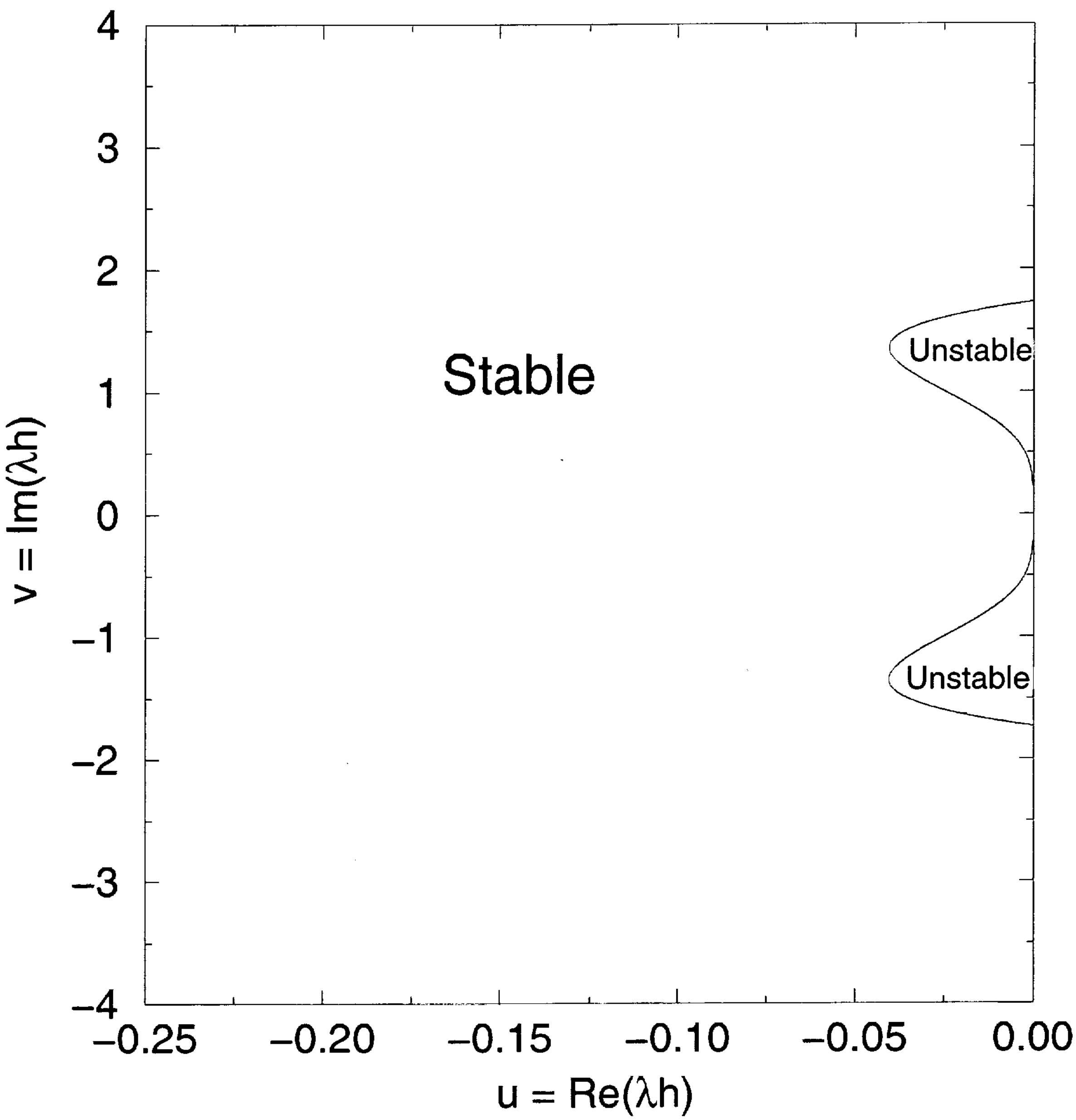

Figure 3   Stability region for a degree-3 fully implicit Taylor series.

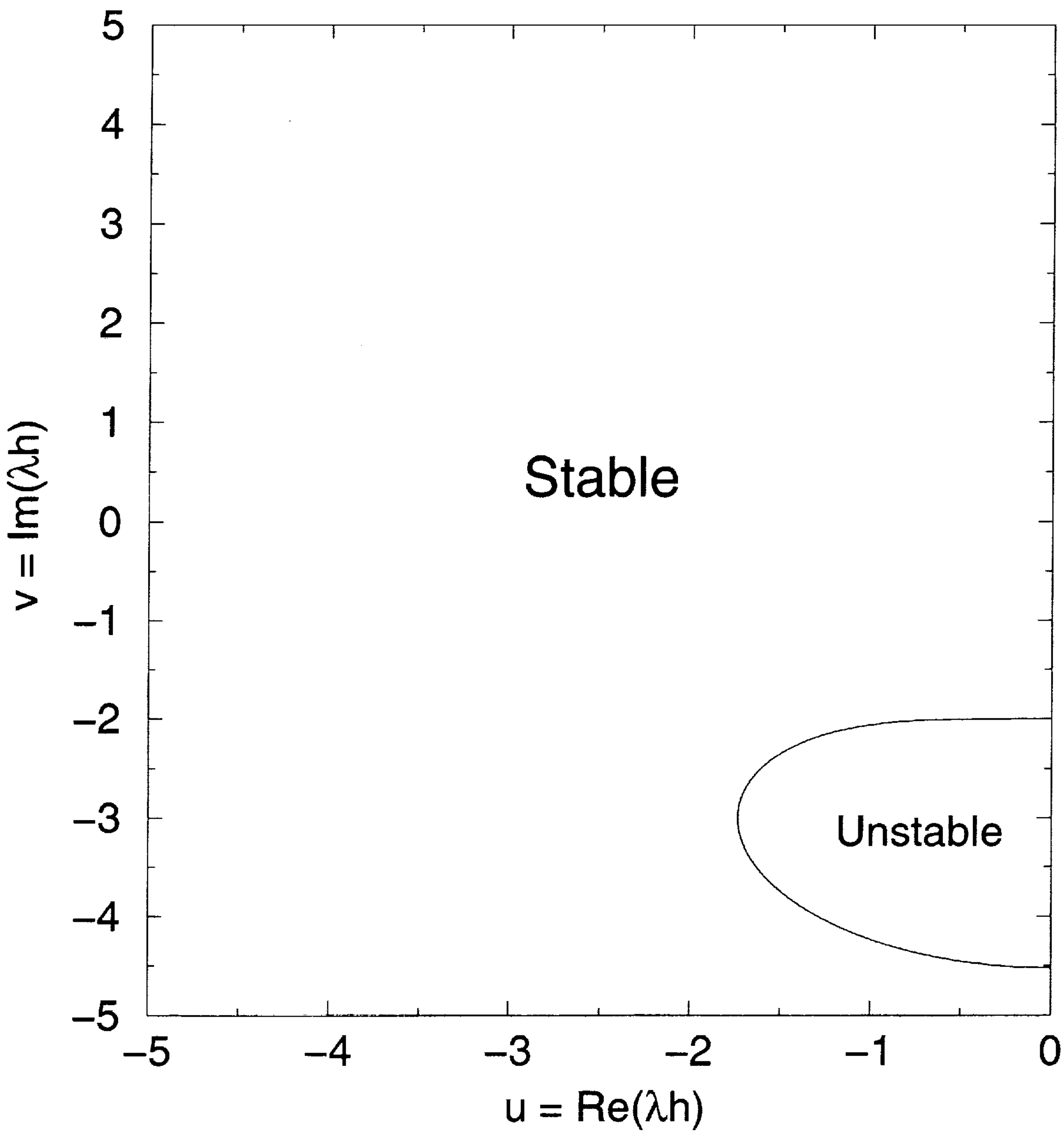

Figure 4.a Stability region for a degree-3 Taylor series with $\mu = \frac{1}{2} + i\,\frac{1}{2}$.

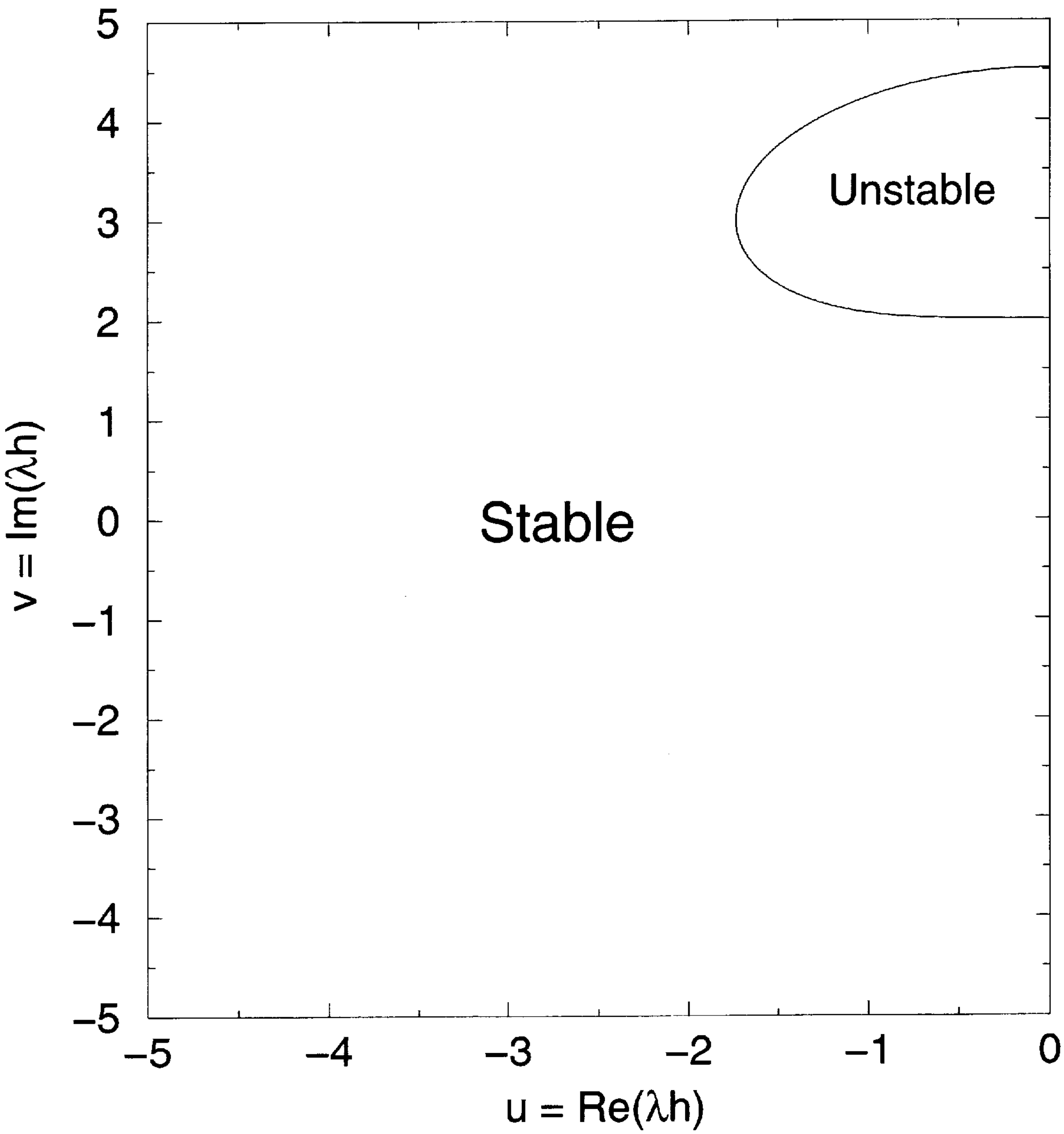

Figure 4.b Stability region for a degree-3 Taylor series with $\mu = \frac{1}{2} - i\,\frac{1}{2}$

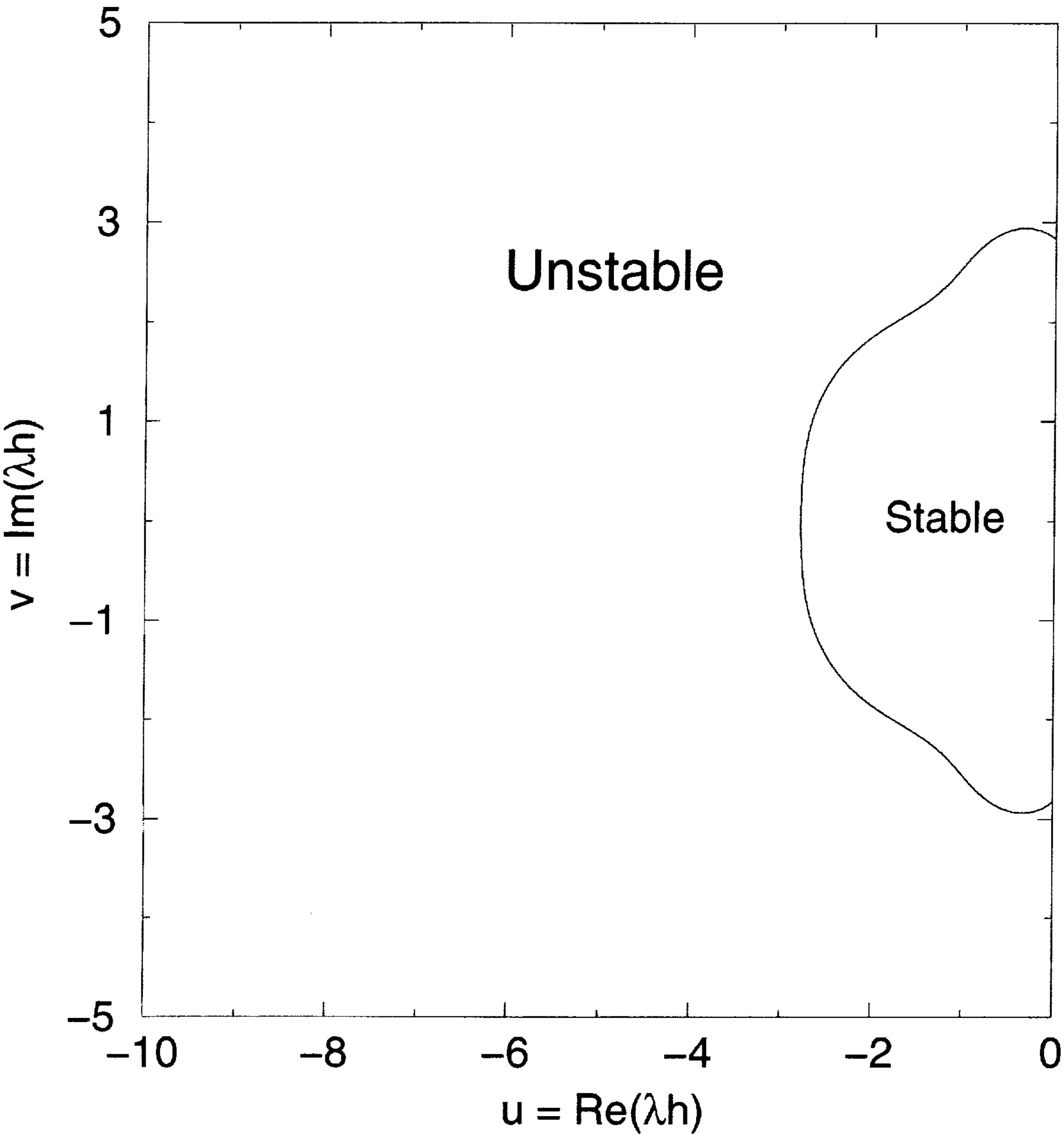

Figure 5   Stability region for a degree-4 explicit Taylor series.

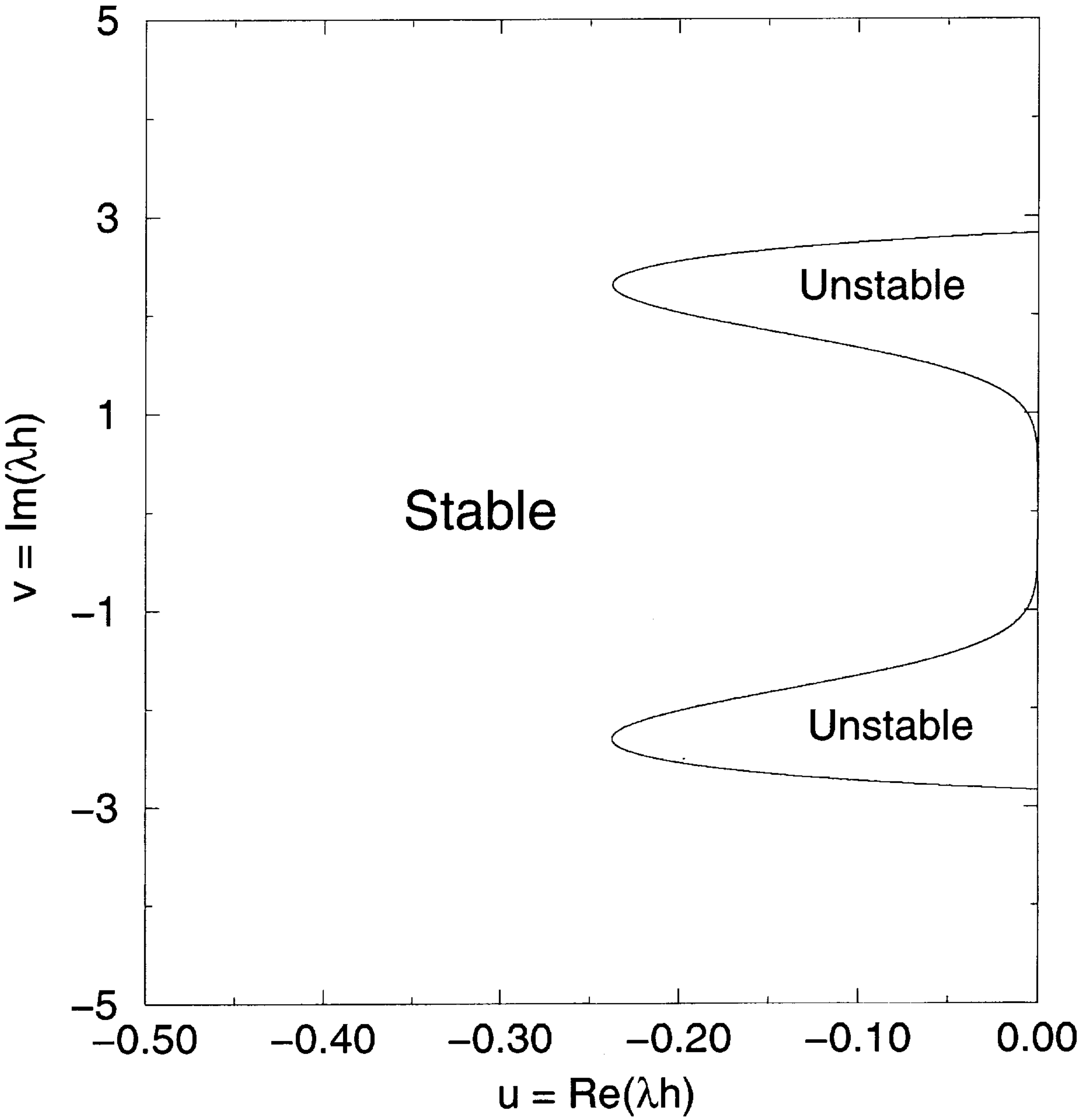

Figure 6 Stability region for a degree-4 fully implicit Taylor series.

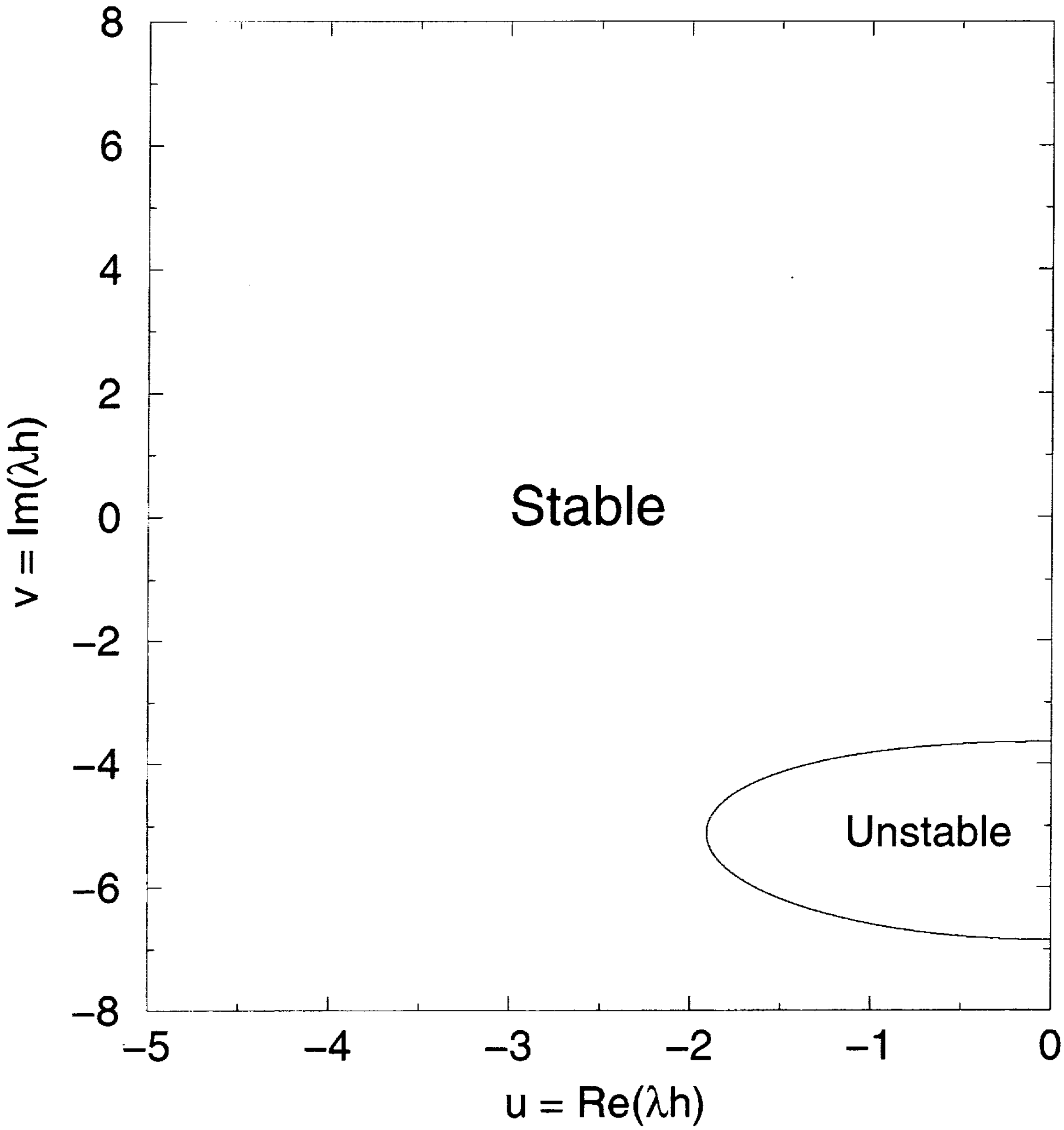

Figure 7.a   Stability region for a degree-4 Taylor series with $\mu = \frac{1}{2} + i\,\frac{1}{2}\,\tan\frac{\pi}{10}$.

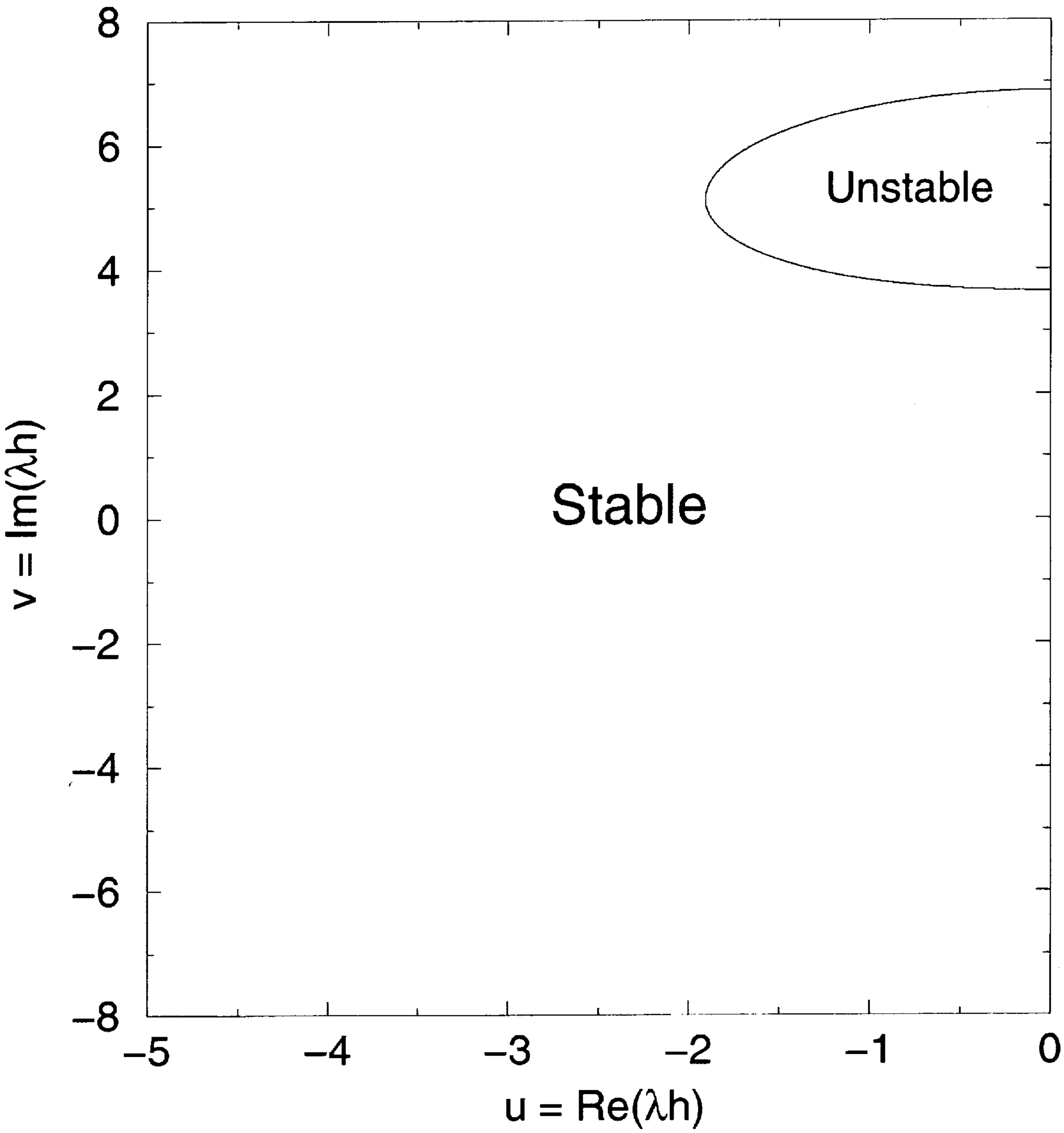

Figure 7.b Stability region for a degree-4 Taylor series with $\mu = \frac{1}{2} - i\,\frac{1}{2}\,\tan\frac{\pi}{10}$.

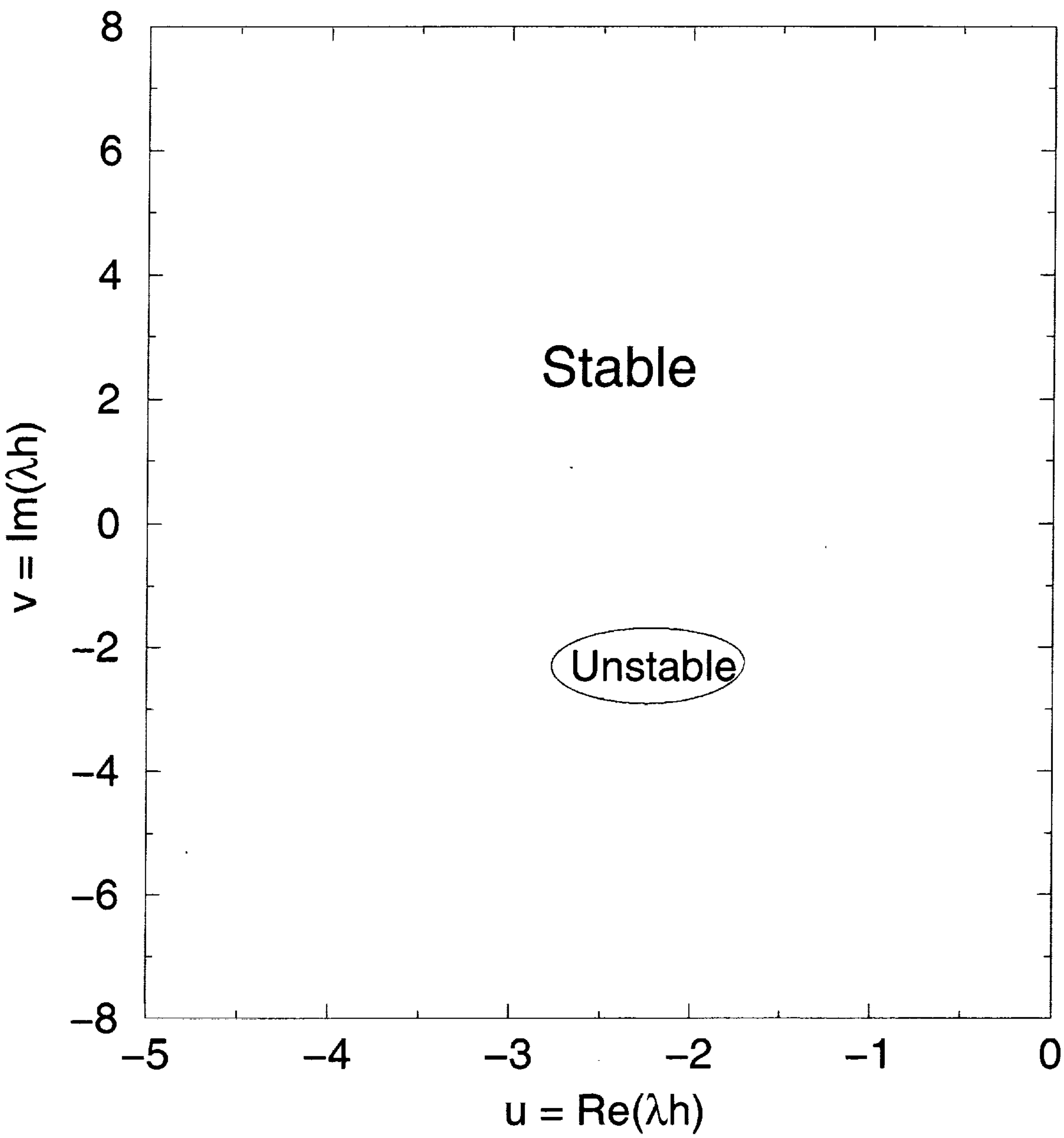

Figure 7.c Stability region for a degree-4 Taylor series with $\mu = \frac{1}{2} + i\,\frac{1}{2}\,\tan\frac{3\pi}{10}$.

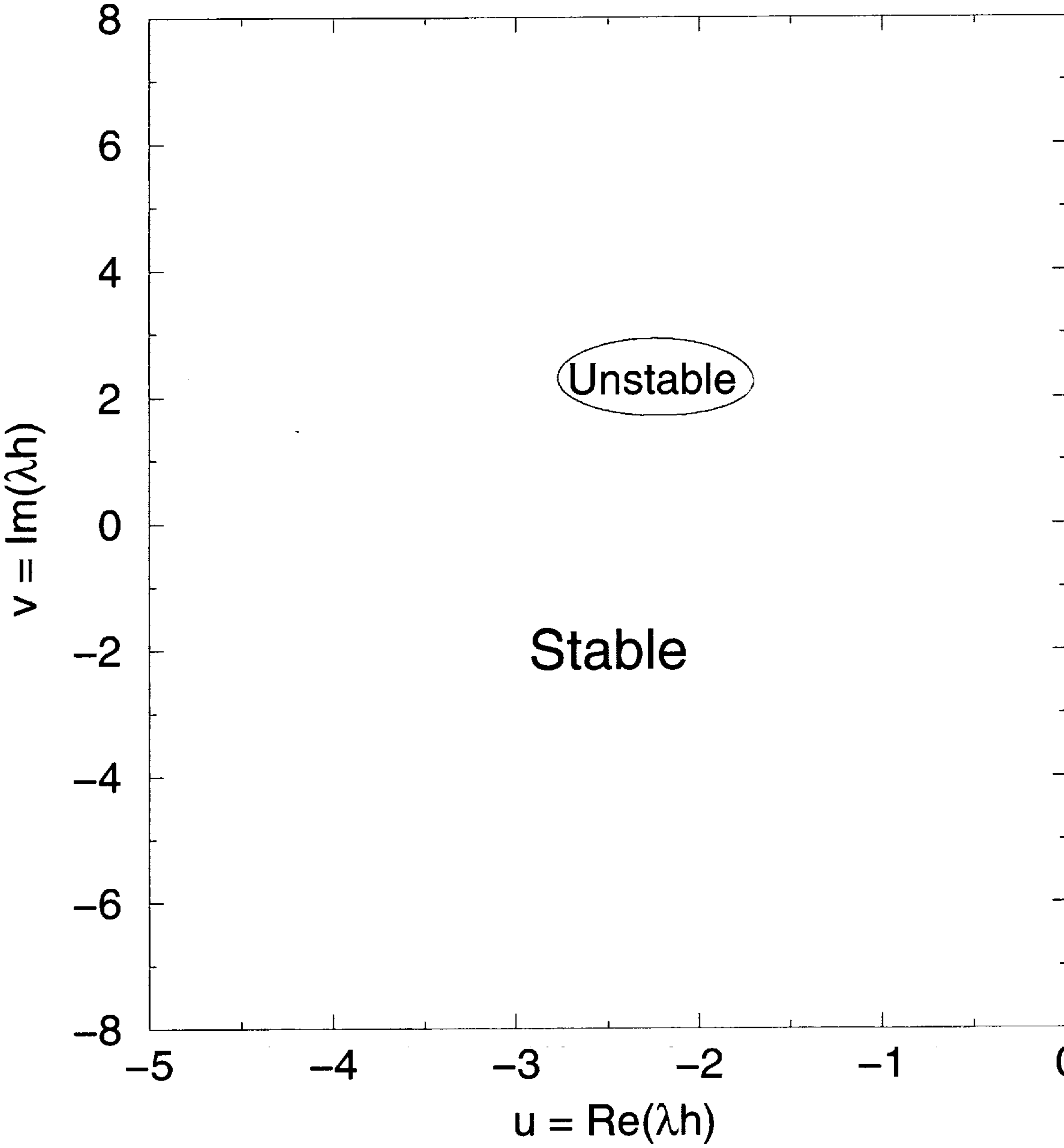

Figure 7.d Stability region for a degree-4 Taylor series with $\mu = \frac{1}{2} - i\,\frac{1}{2}\,\tan\frac{3\pi}{10}$.

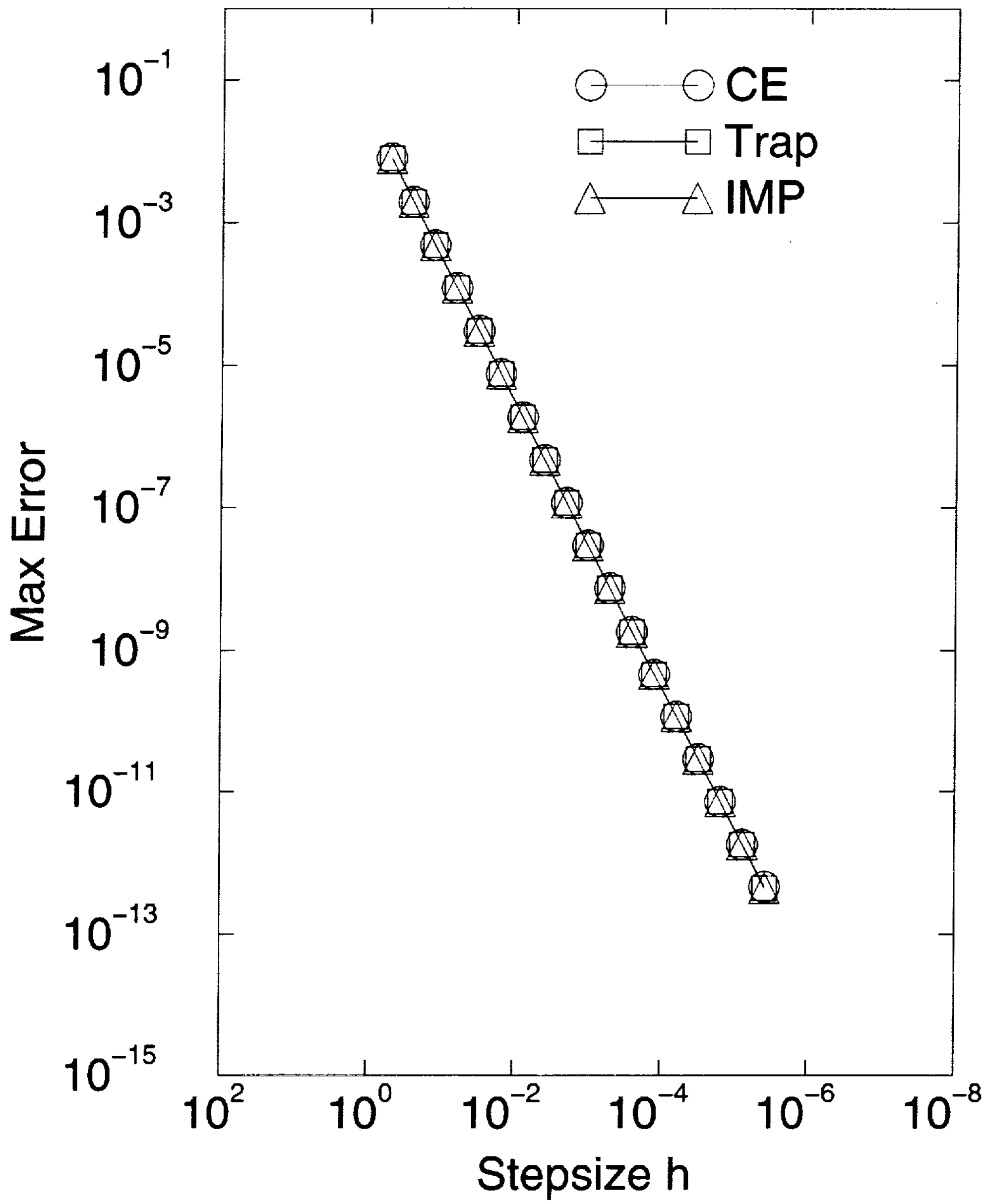

Figure 8.a Reduction of error for Problem 1. Results are shown for the Centered Euler Method, Trapezoidal Rule, and Implicit Midpoint Rule.

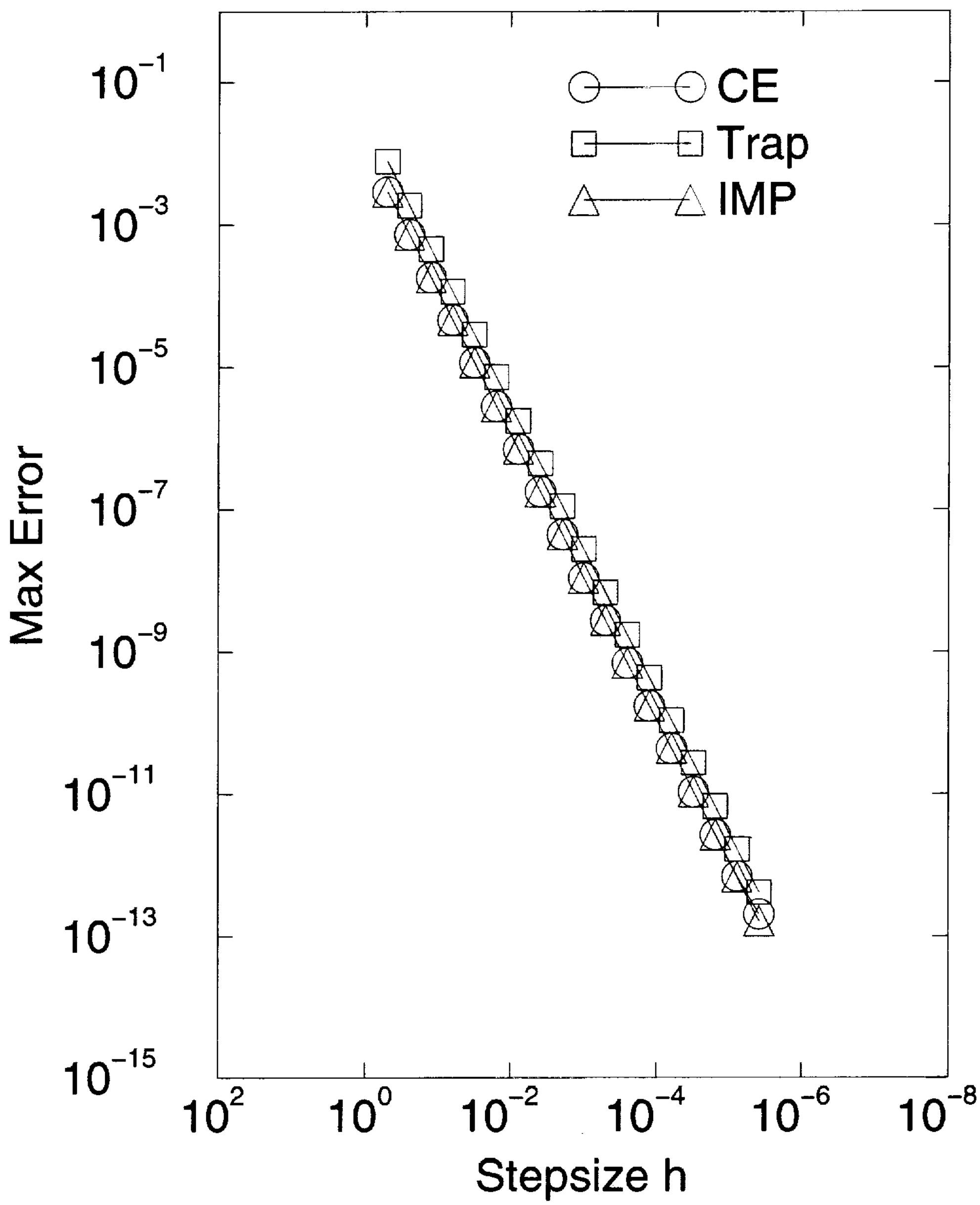

Figure 8.b Reduction of error for Problem 2. Results are shown for the Centered Euler Method, Trapezoidal Rule, and Implicit Midpoint Rule.

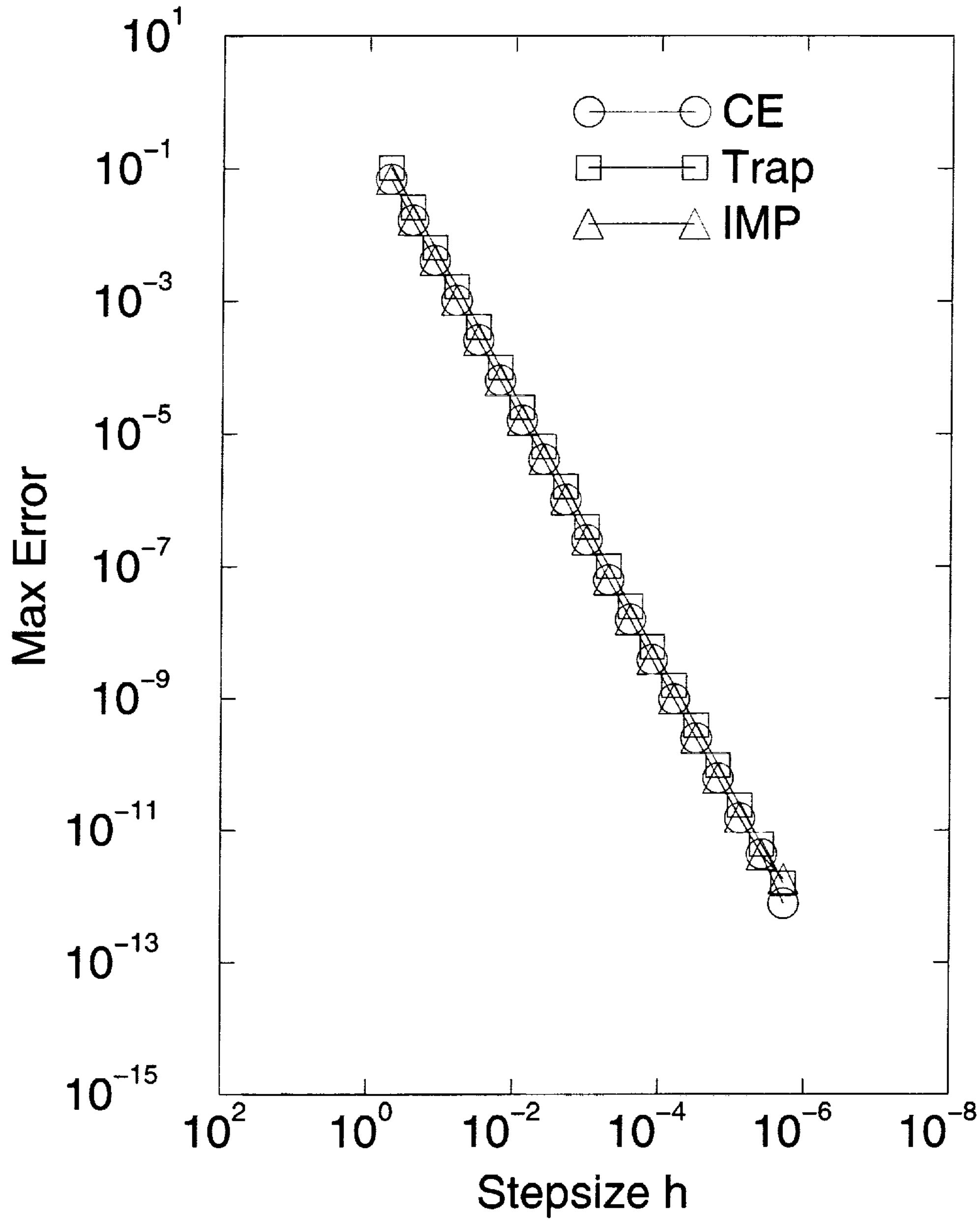

Figure 8.c Reduction of error for Problem 3. Results are shown for the Centered Euler Method, Trapezoidal Rule, and Implicit Midpoint Rule.

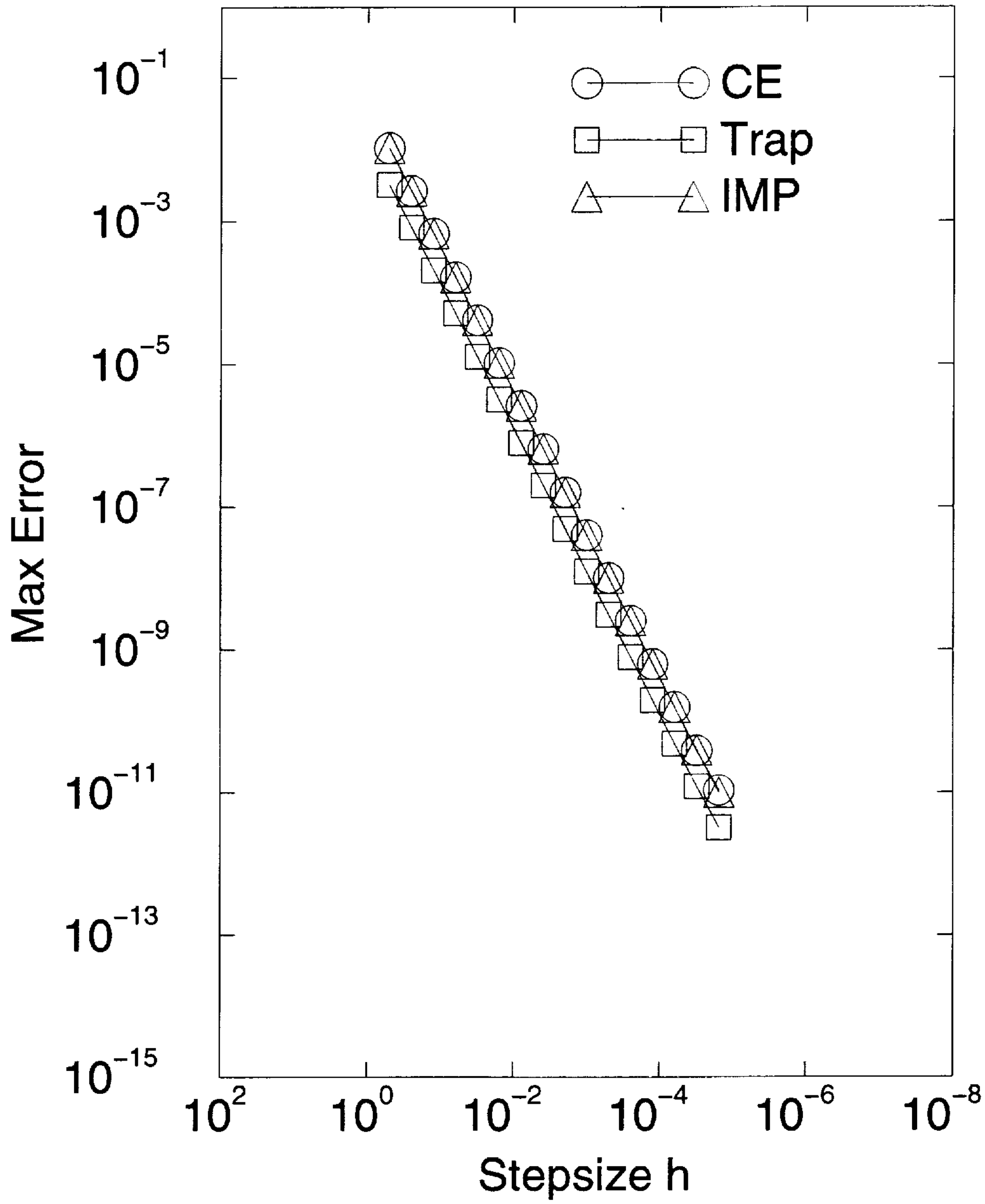

Figure 8.d Reduction of error for Problem 4. Results are shown for the Centered Euler Method, Trapezoidal Rule, and Implicit Midpoint Rule.

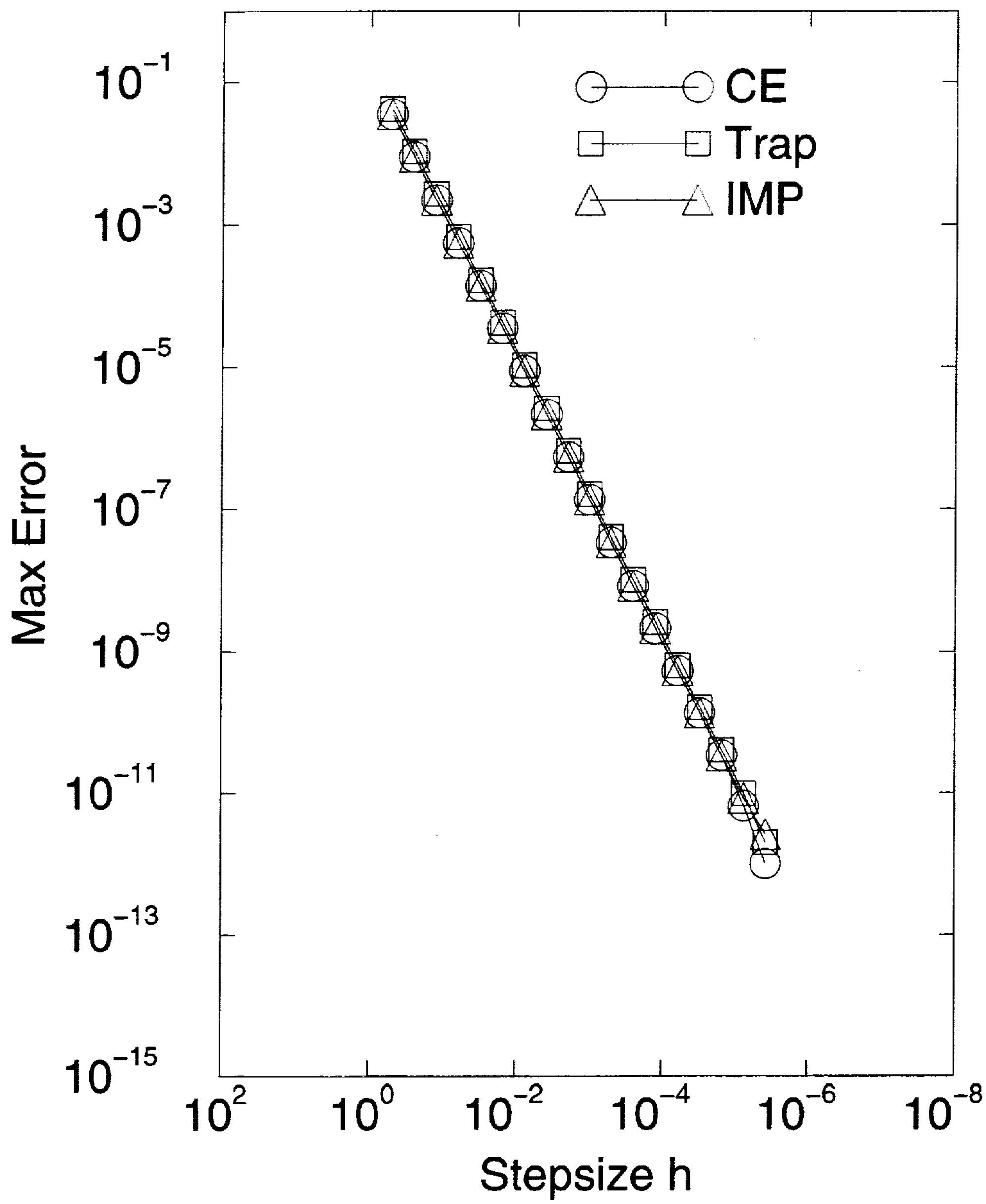

Figure 8.e Reduction of error for Problem 5. Results are shown for the Centered Euler Method, Trapezoidal Rule, and Implicit Midpoint Rule.

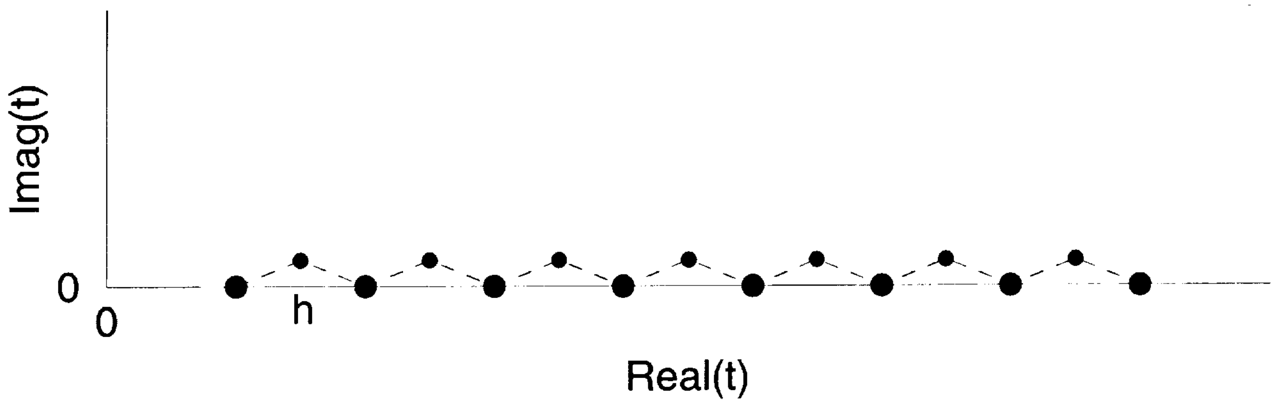

Figure 9 Integration path for a degree-2 Taylor series with $\mu = \frac{1}{2} + i\,\frac{\sqrt{3}}{6}$.

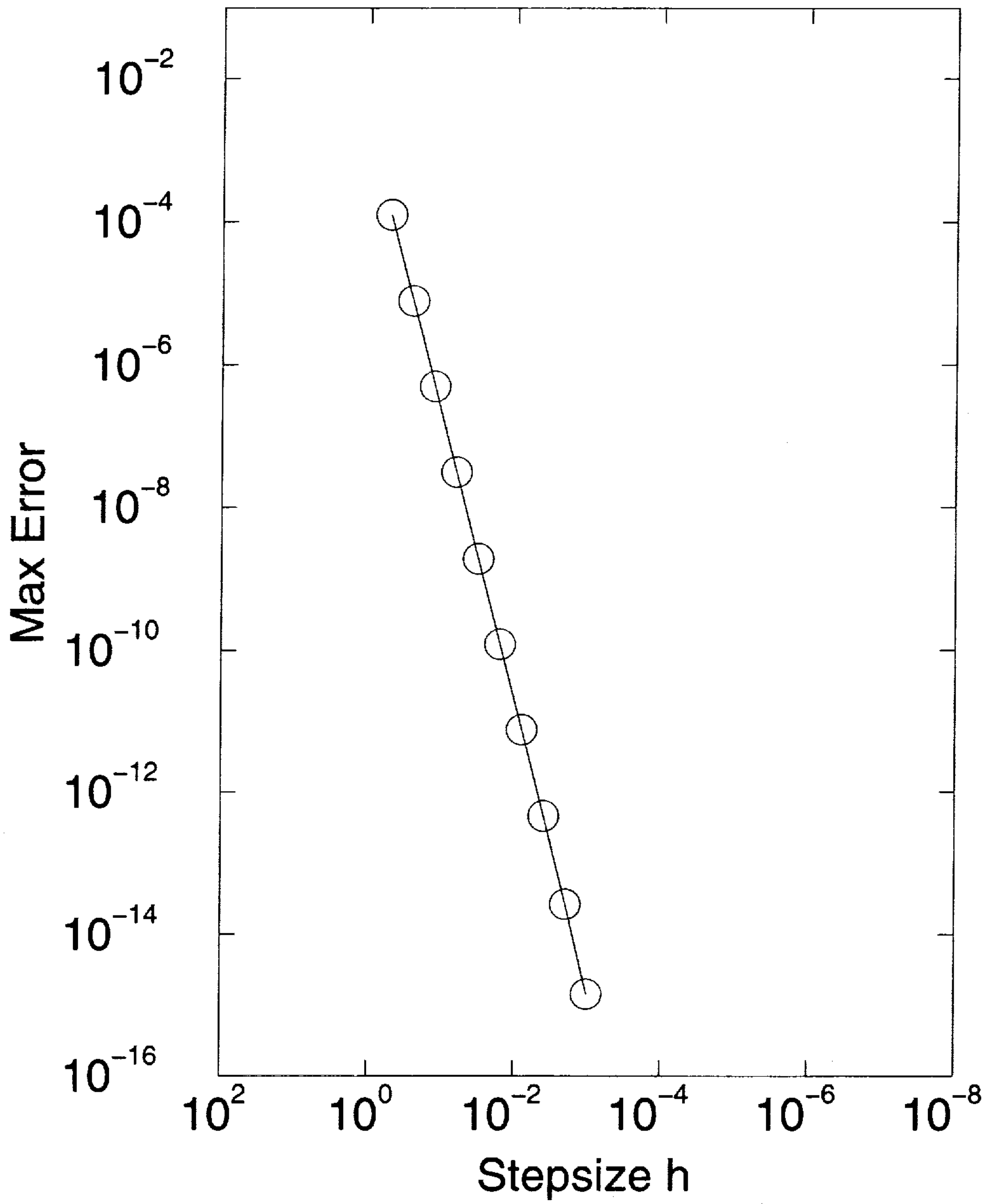

Figure 10.a Reduction of error for Problem 1 using a degree-2 Taylor series with $\mu = \frac{1}{2} + i\frac{\sqrt{3}}{6}$.

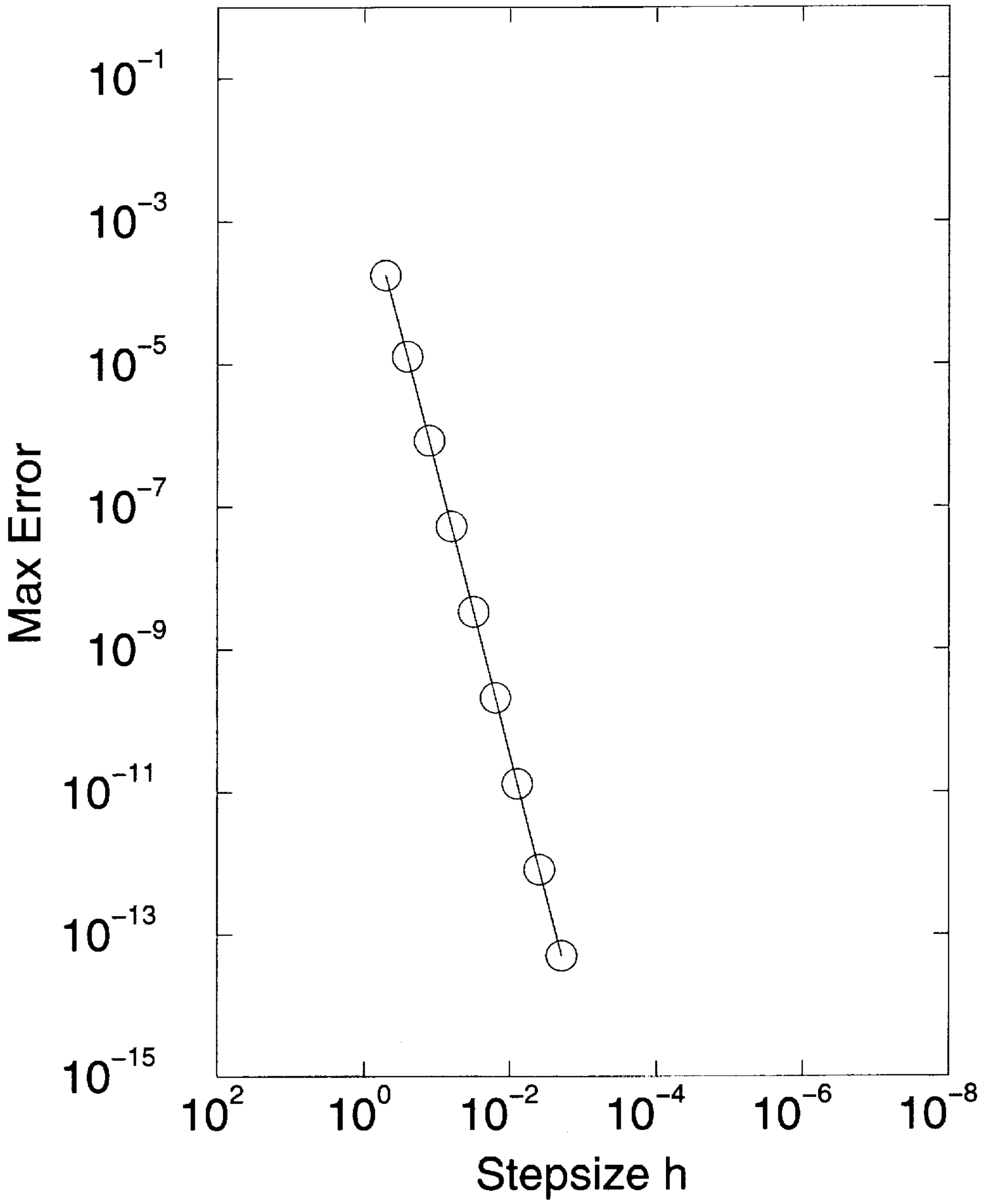

Figure 10.b Reduction of error for Problem 2 using a degree-2 Taylor series with $\mu = \frac{1}{2} + i\,\frac{\sqrt{3}}{6}$.

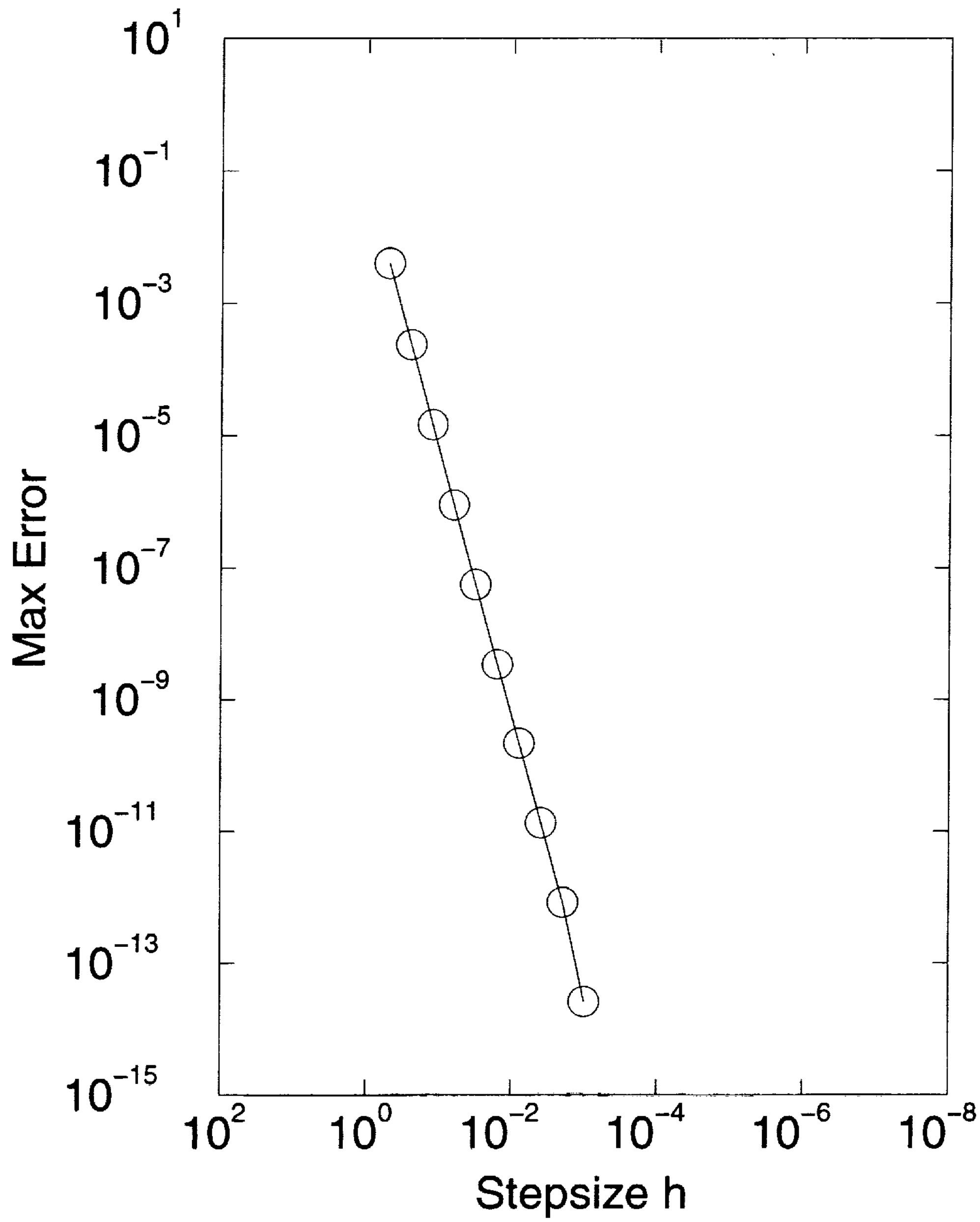

Figure 10.c Reduction of error for Problem 3 using a degree-2 Taylor series with $\mu = \frac{1}{2} + i\frac{\sqrt{3}}{6}$.

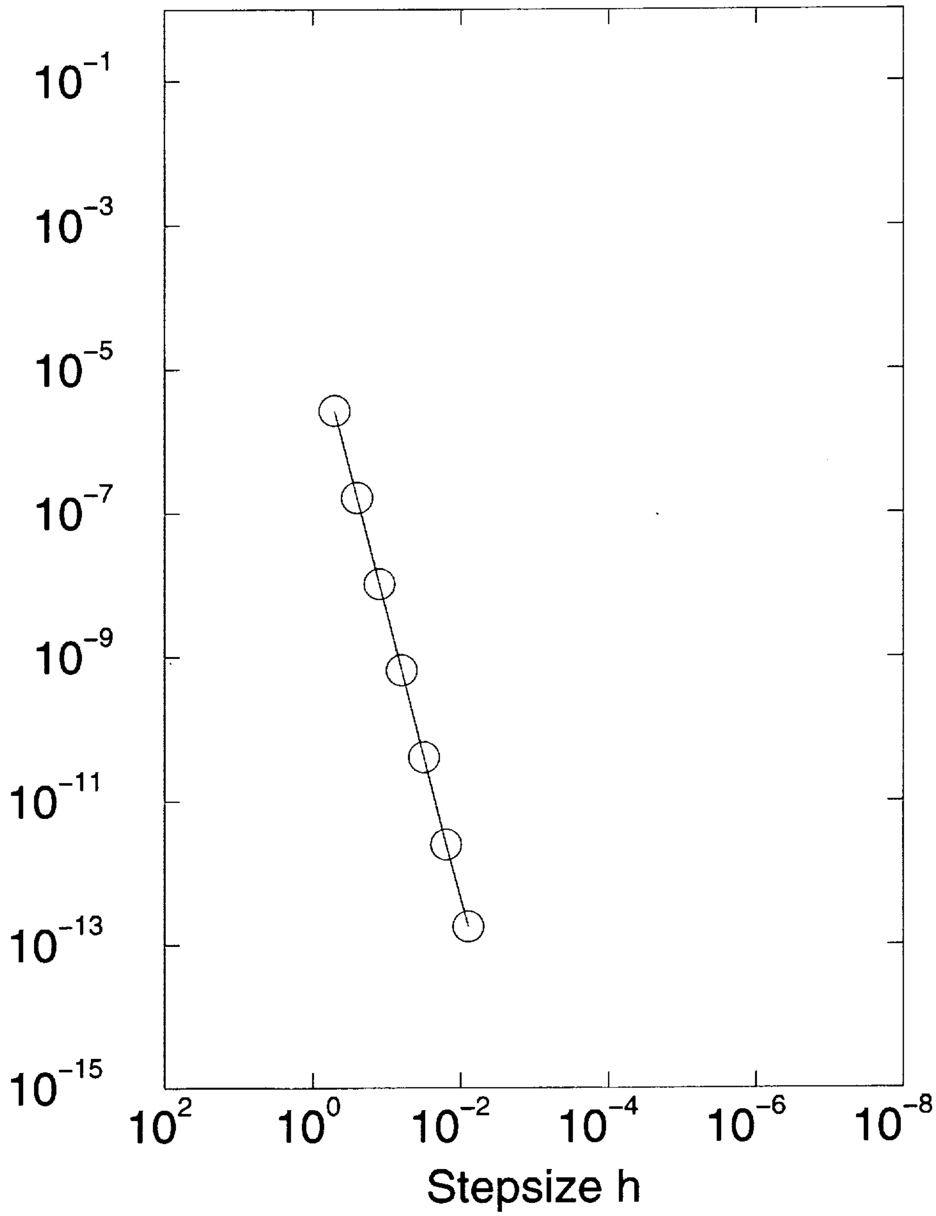

Figure 10.d Reduction of error for Problem 4 using a degree-2 Taylor series with $\mu = \frac{1}{2} + i\frac{\sqrt{3}}{6}$.

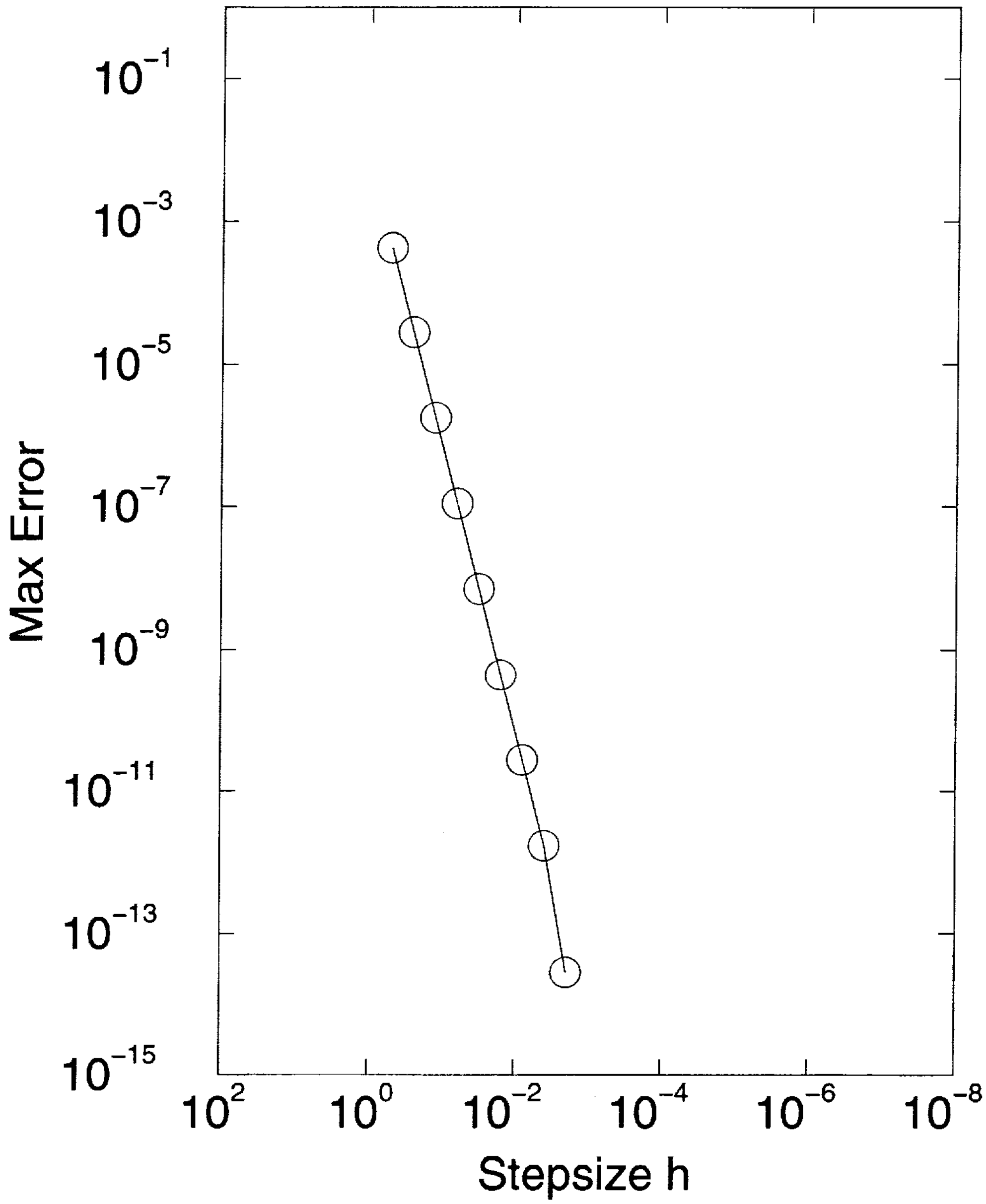

Figure 10.e Reduction of error for Problem 5 using a degree-2 Taylor series with $\mu = \frac{1}{2} + i\frac{\sqrt{3}}{6}$.

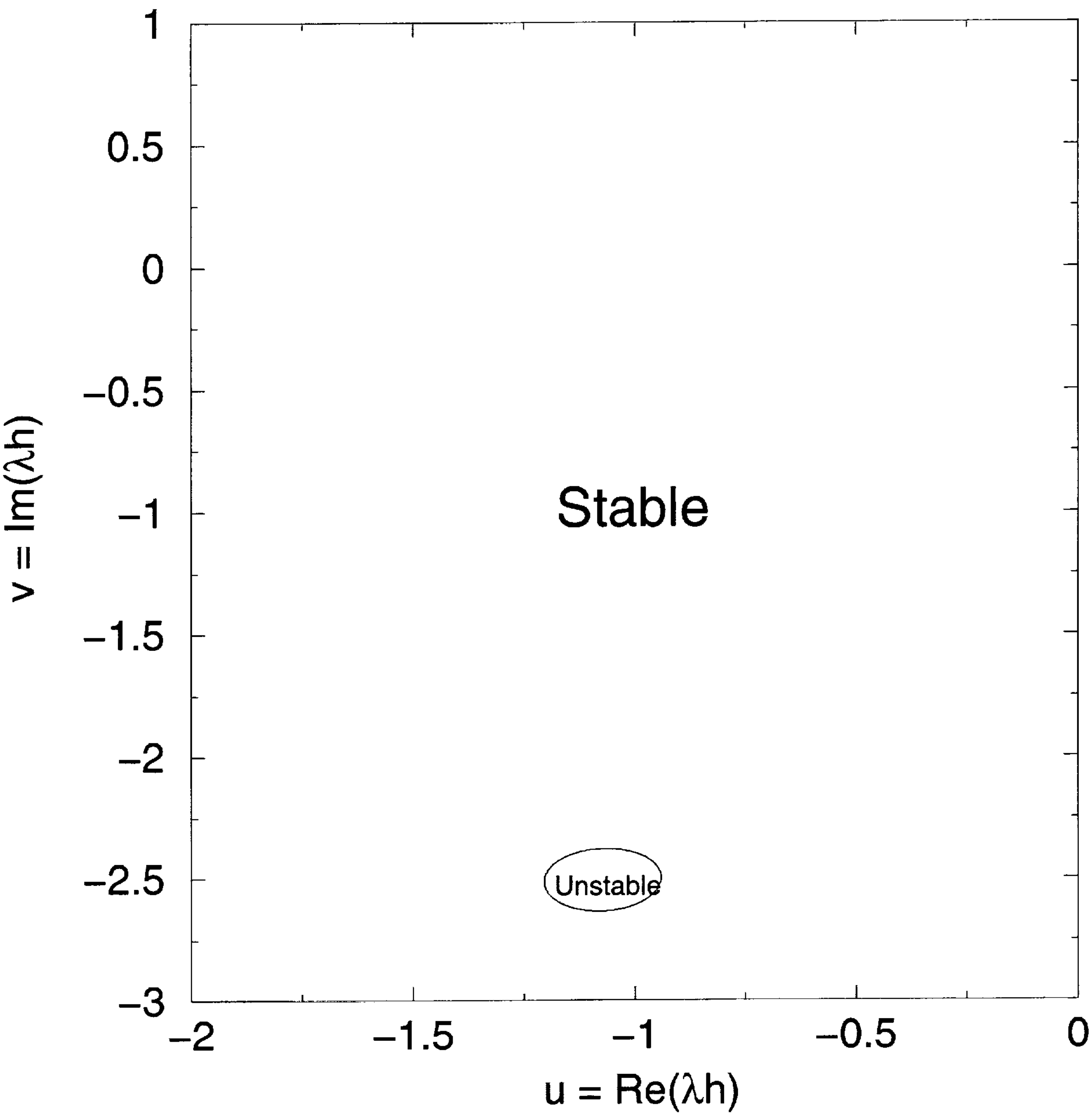

Figure 11 Stability region for a degree-3 Taylor series with extrapolation.

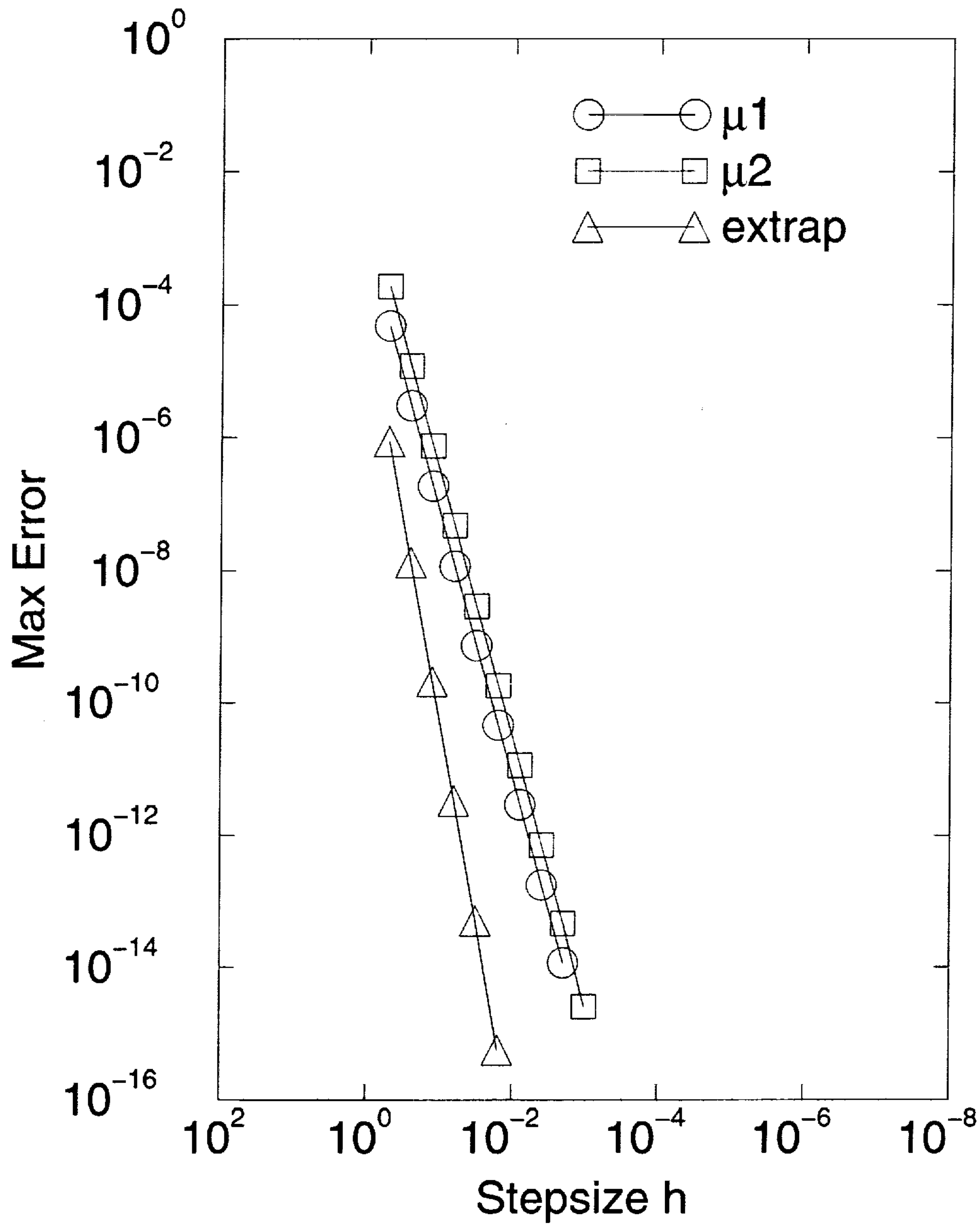

Figure 12.a Reduction of error for Problem 1 using a degree-3 Taylor series with $\mu_1 = \frac{1}{2}$, $\mu_2 = \frac{1}{2} + i\,\frac{1}{2}$, and with extrapolation.

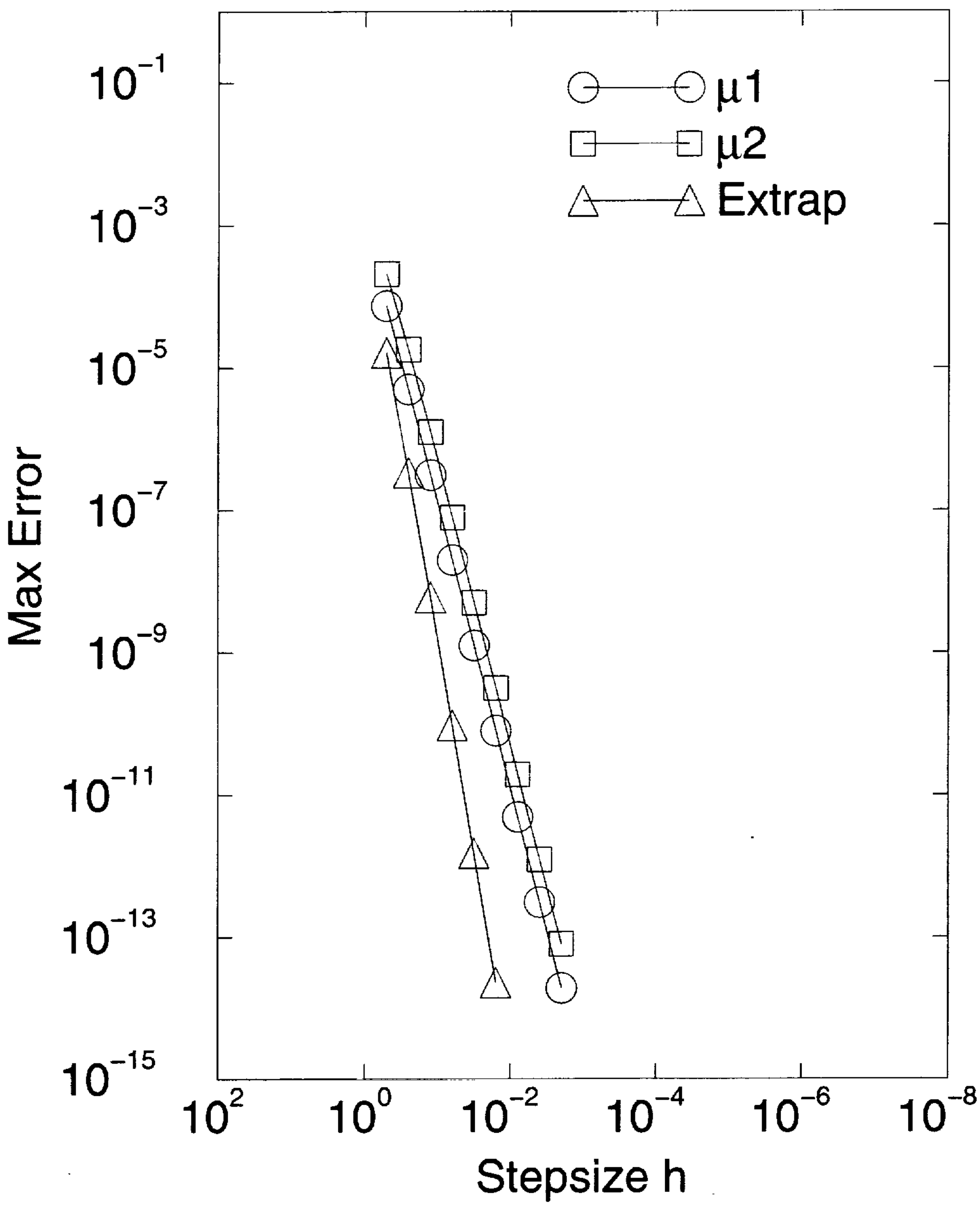

Figure 12.b Reduction of error for Problem 2 using a degree-3 Taylor series with $\mu_1 = \frac{1}{2}$, $\mu_2 = \frac{1}{2} + i\,\frac{1}{2}$, and with extrapolation.

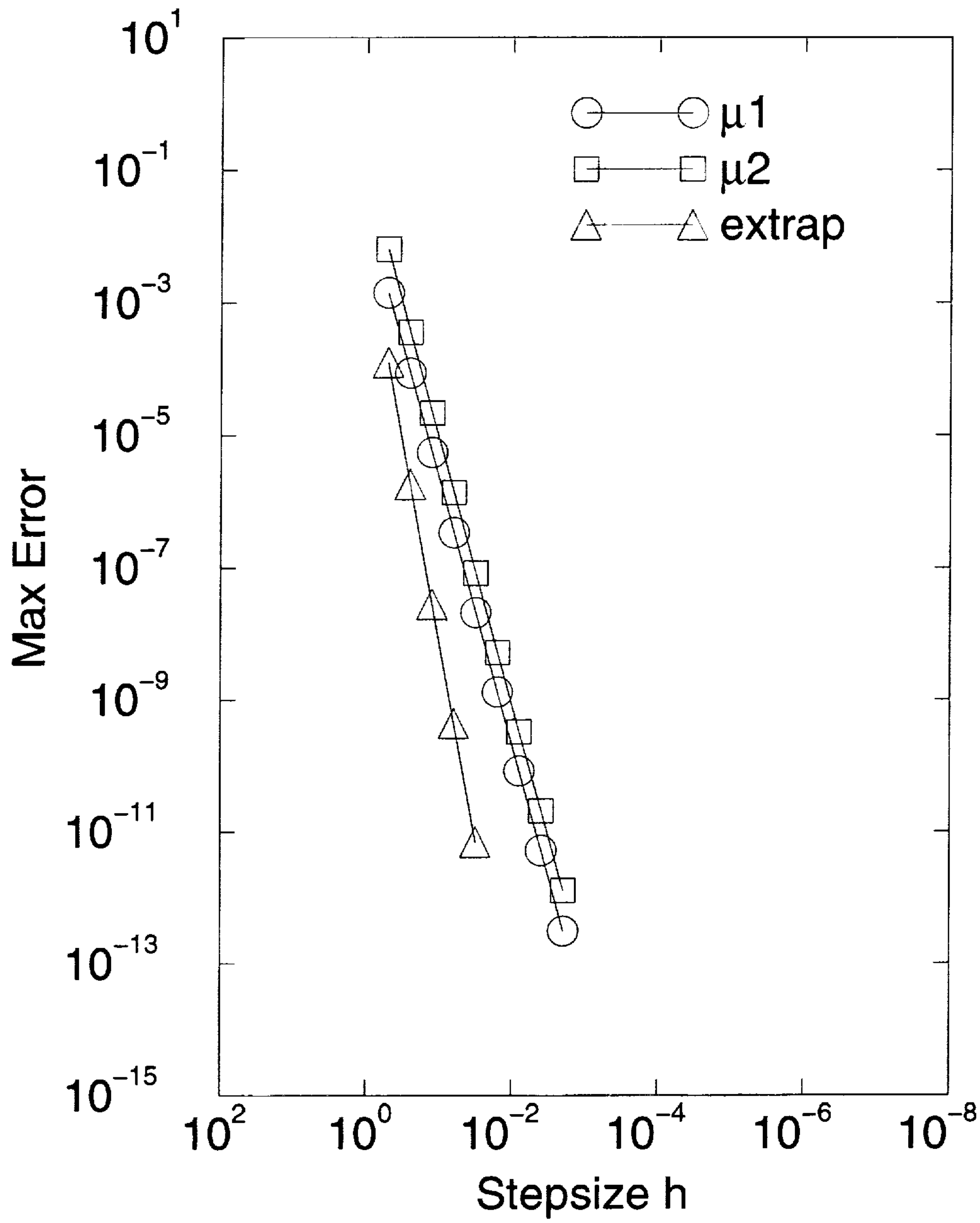

Figure 12.c Reduction of error for Problem 3 using a degree-3 Taylor series with $\mu_1 = \frac{1}{2}$, $\mu_2 = \frac{1}{2} + i\,\frac{1}{2}$, and with extrapolation.

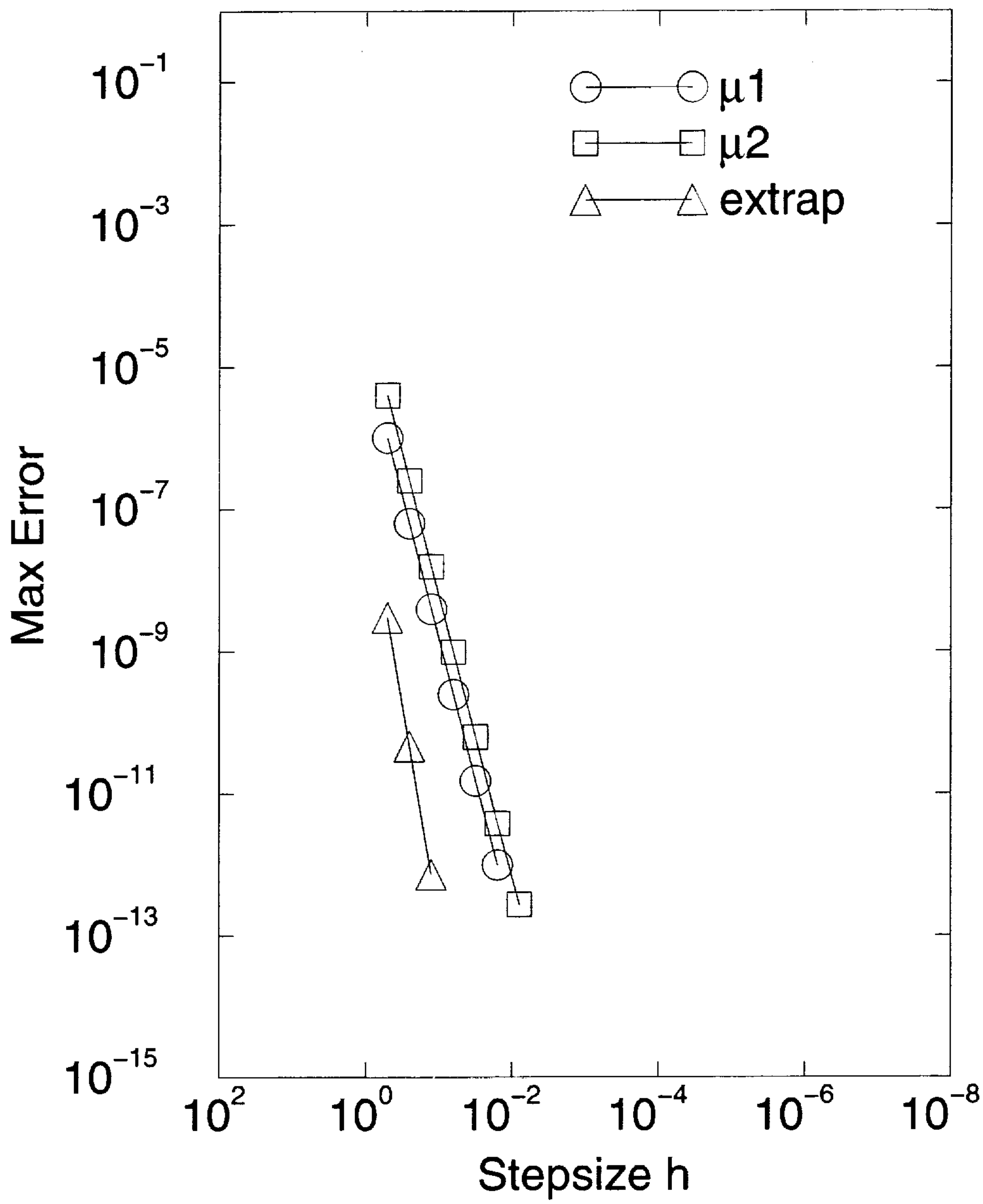

Figure 12.d Reduction of error for Problem 4 using a degree-3 Taylor series with $\mu_1 = \frac{1}{2}$, $\mu_2 = \frac{1}{2} + i\,\frac{1}{2}$, and with extrapolation.

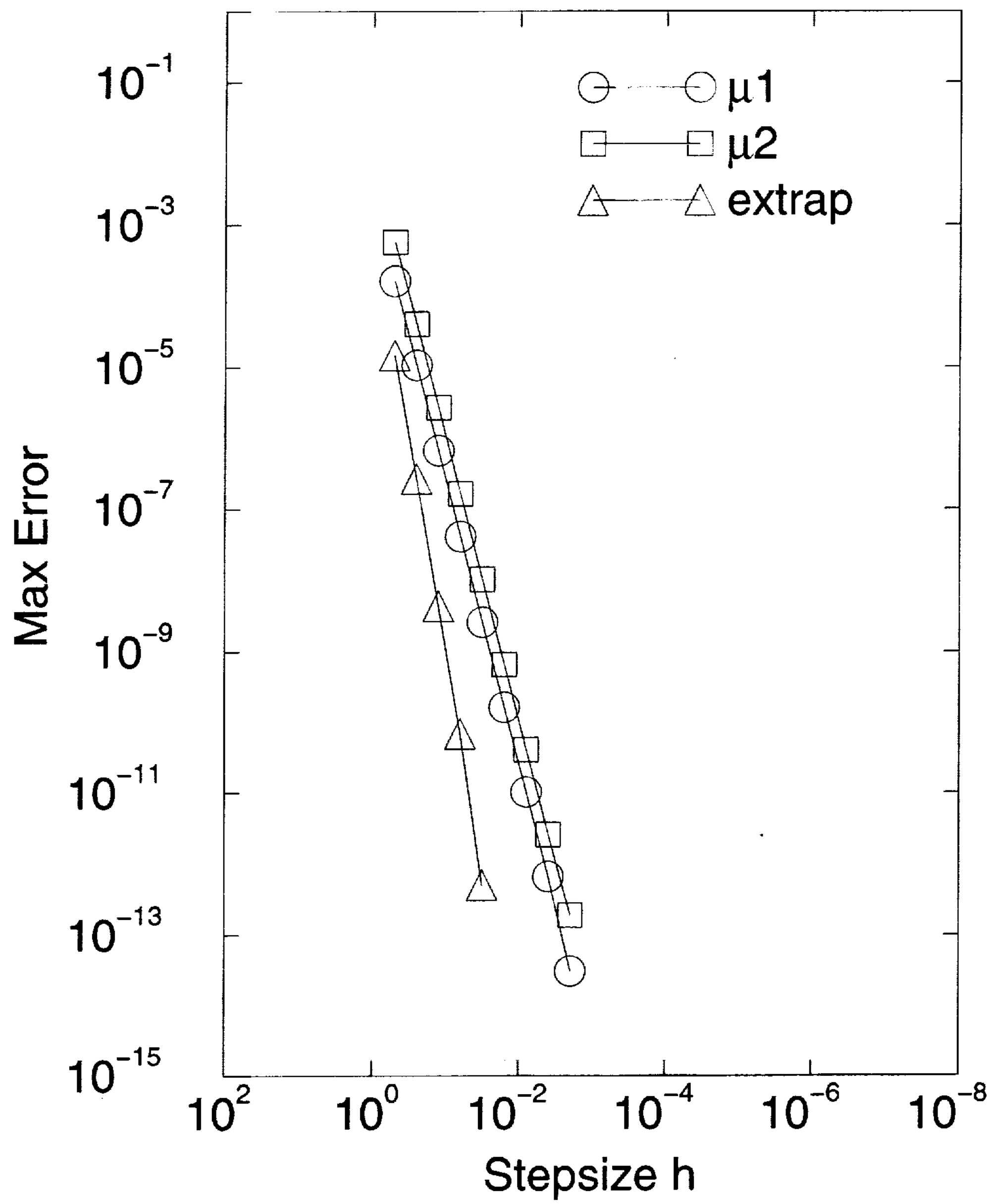

Figure 12.e Reduction of error for Problem 5 using a degree-3 Taylor series with $\mu_1 = \frac{1}{2}$, $\mu_2 = \frac{1}{2} + i\,\frac{1}{2}$, and with extrapolation.

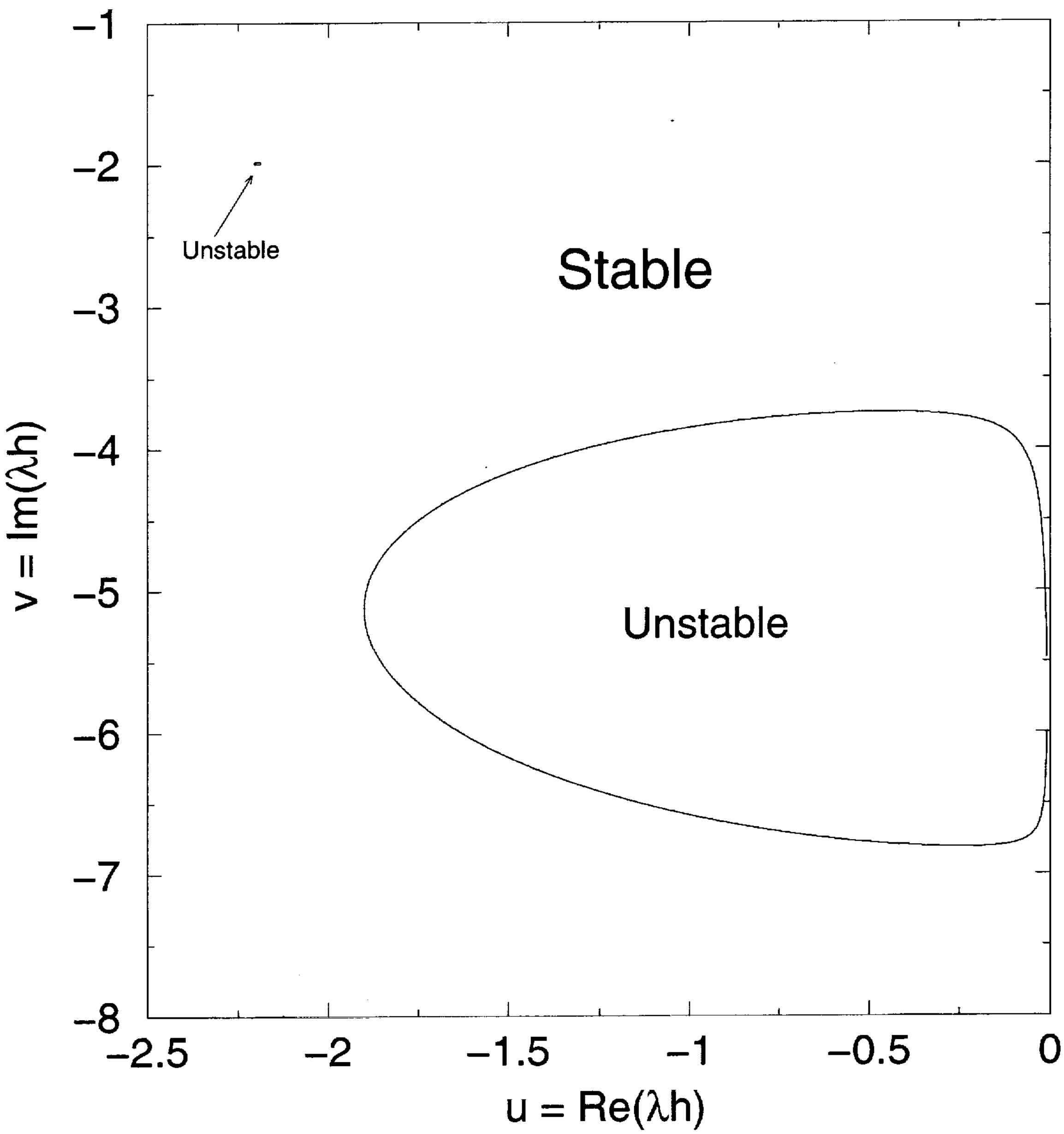

Figure 13   Stability region for a degree-4 Taylor series with extrapolation.

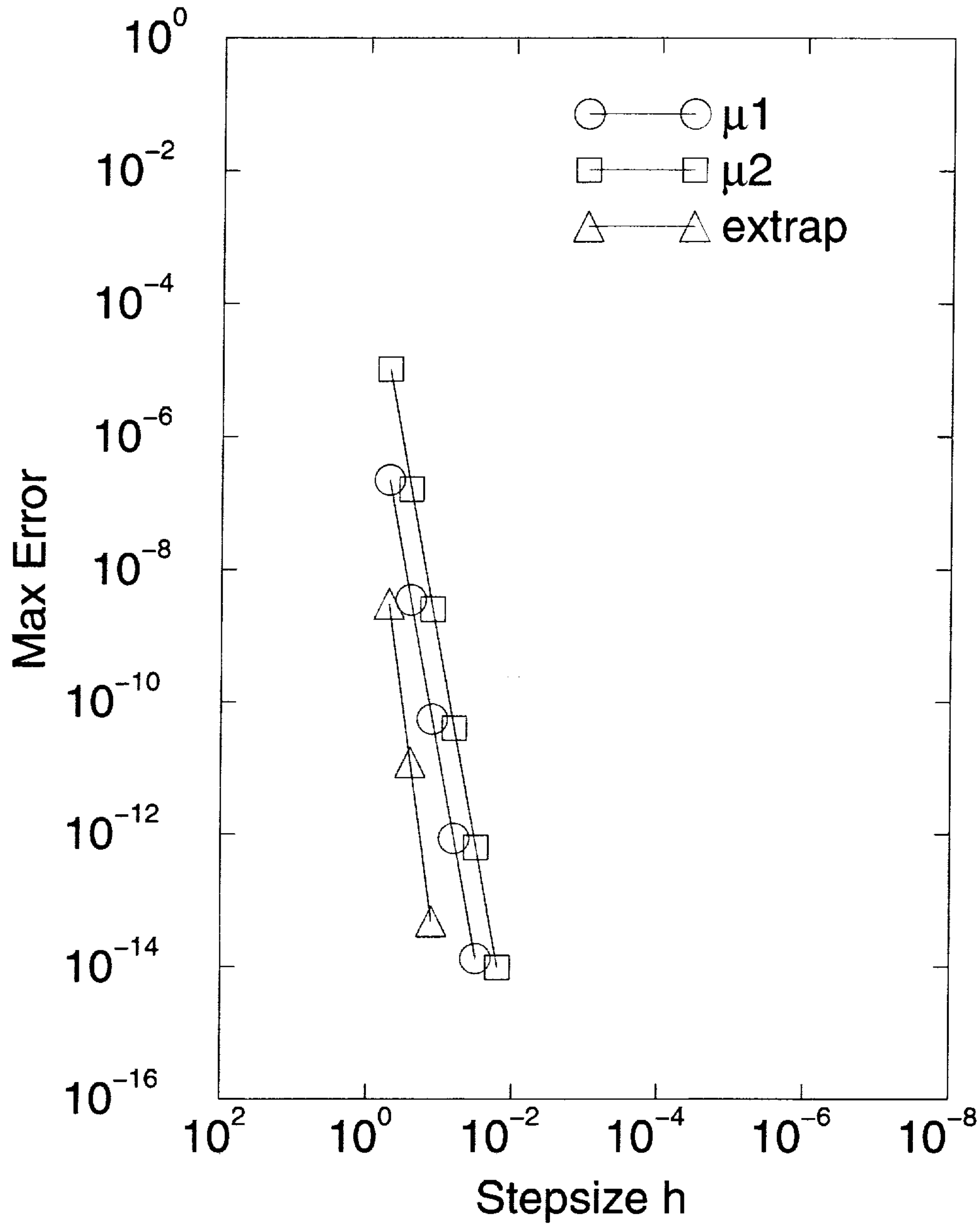

Figure 14.a Reduction of error for Problem 1 using a degree-4 Taylor series with $\mu_1 = \frac{1}{2} + i\,\frac{1}{2}\tan\frac{\pi}{10}$, $\mu_2 = \frac{1}{2} + i\,\frac{1}{2}\tan\frac{3\pi}{10}$, and with extrapolation.

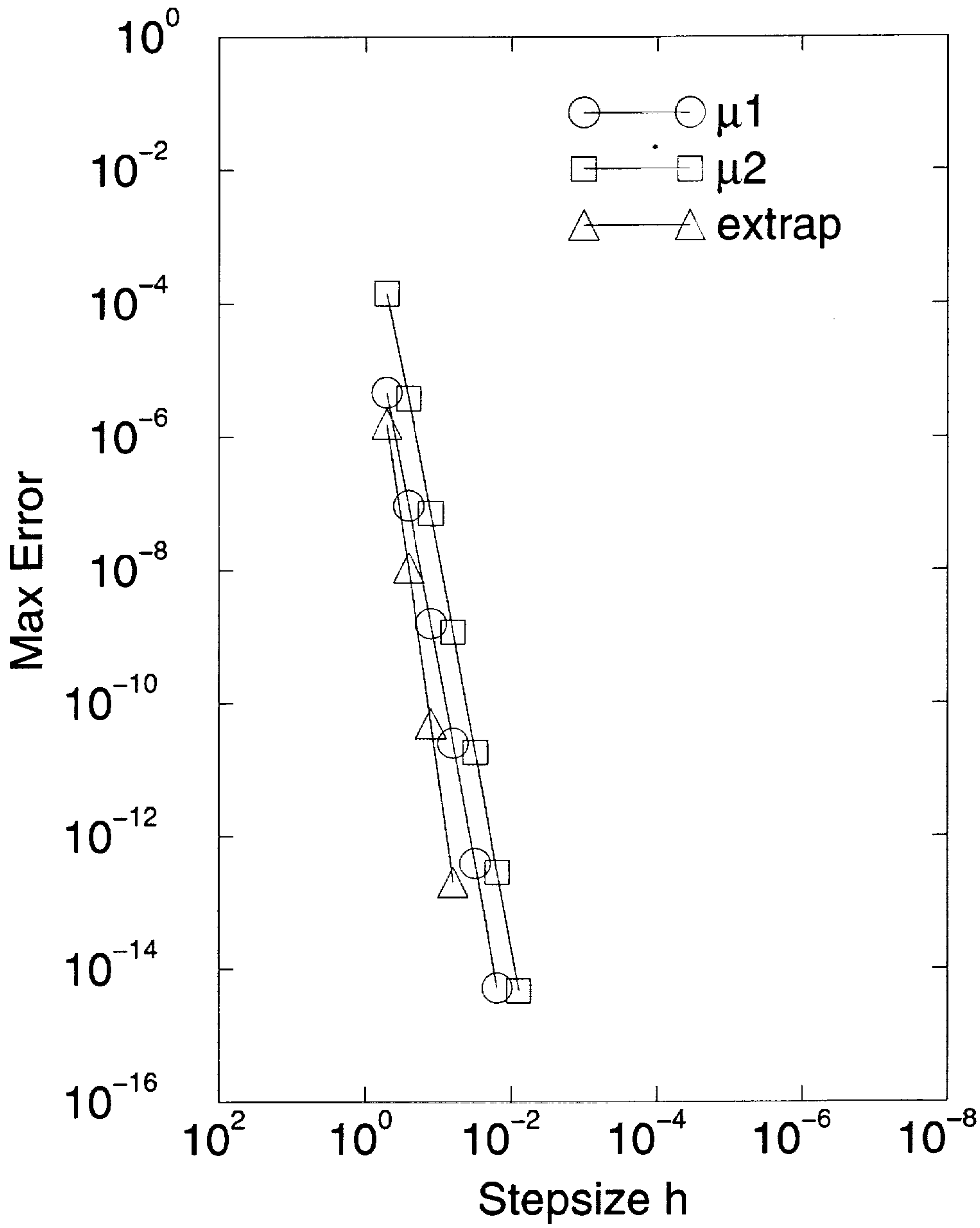

Figure 14.b Reduction of error for Problem 2 using a degree-4 Taylor series with $\mu_1 = \frac{1}{2} + i\frac{1}{2}\tan\frac{\pi}{10}$, $\mu_2 = \frac{1}{2} + i\frac{1}{2}\tan\frac{3\pi}{10}$, and with extrapolation.

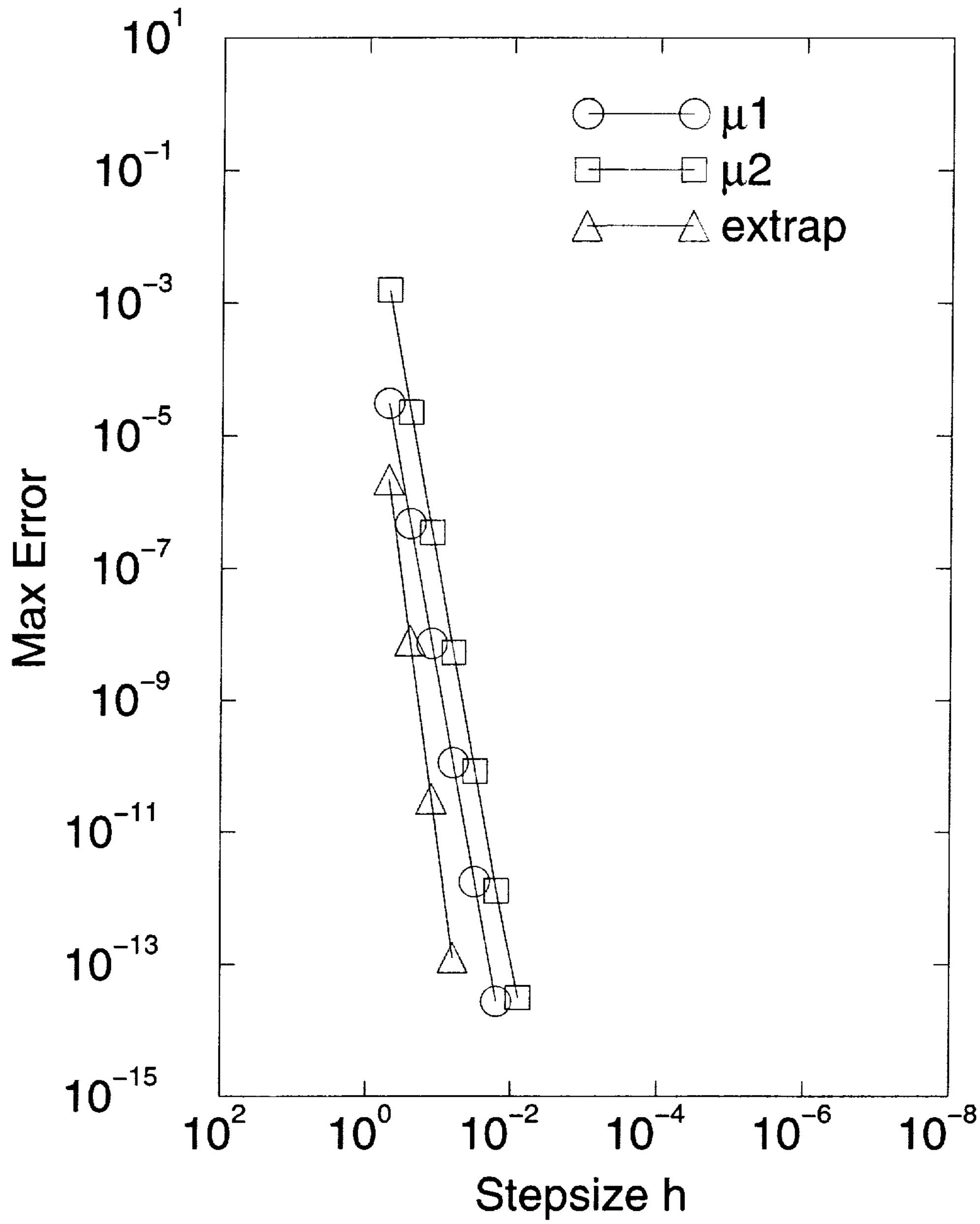

Figure 14.c Reduction of error for Problem 3 using a degree-4 Taylor series with $\mu_1 = \frac{1}{2} + i\,\frac{1}{2}\tan\frac{\pi}{10}$, $\mu_2 = \frac{1}{2} + i\,\frac{1}{2}\tan\frac{3\pi}{10}$, and with extrapolation.

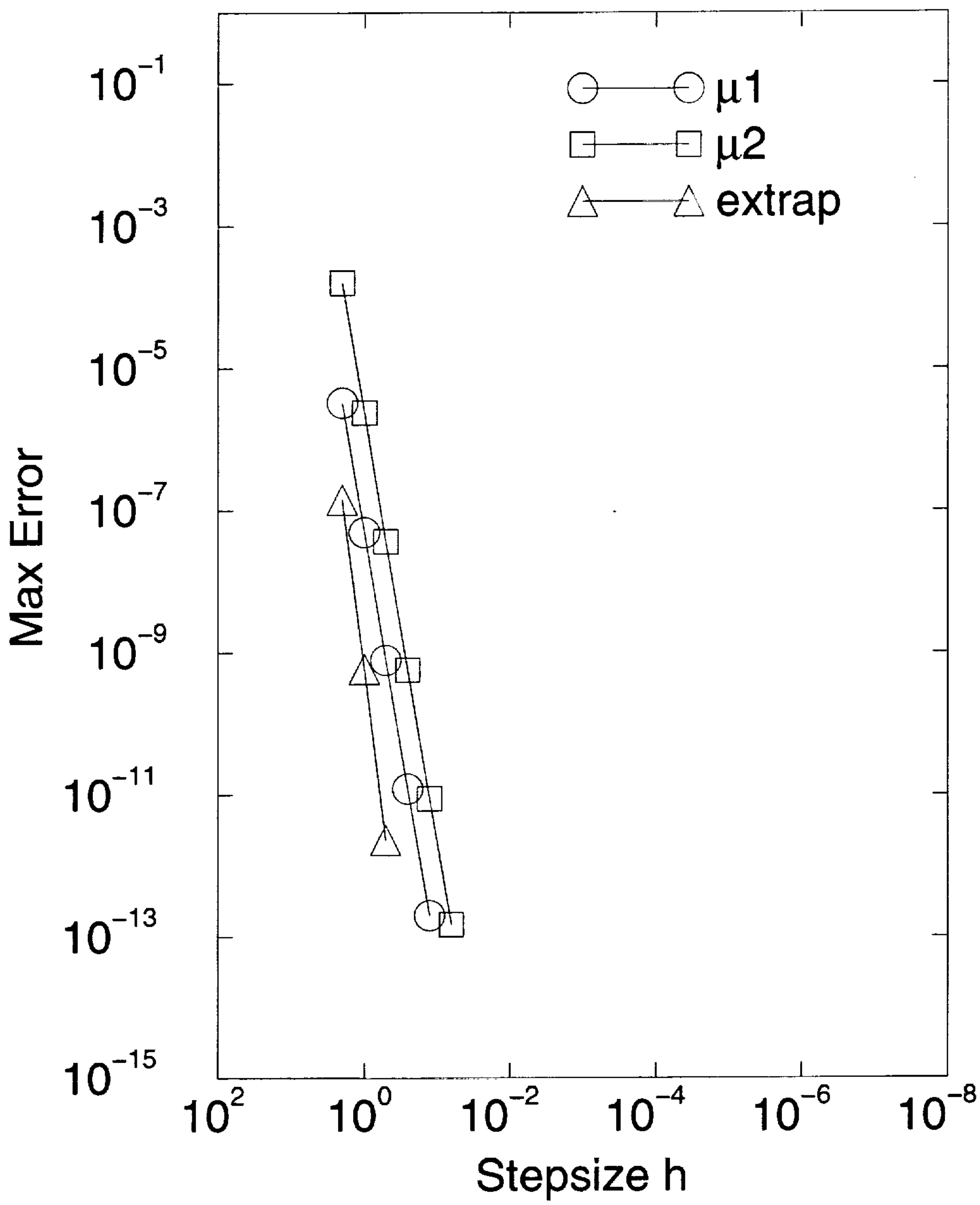

Figure 14.d Reduction of error for Problem 4 using a degree-4 Taylor series with $\mu_1 = \frac{1}{2} + i\,\frac{1}{2}\,\tan\frac{\pi}{10}$, $\mu_2 = \frac{1}{2} + i\,\frac{1}{2}\,\tan\frac{3\pi}{10}$, and with extrapolation.

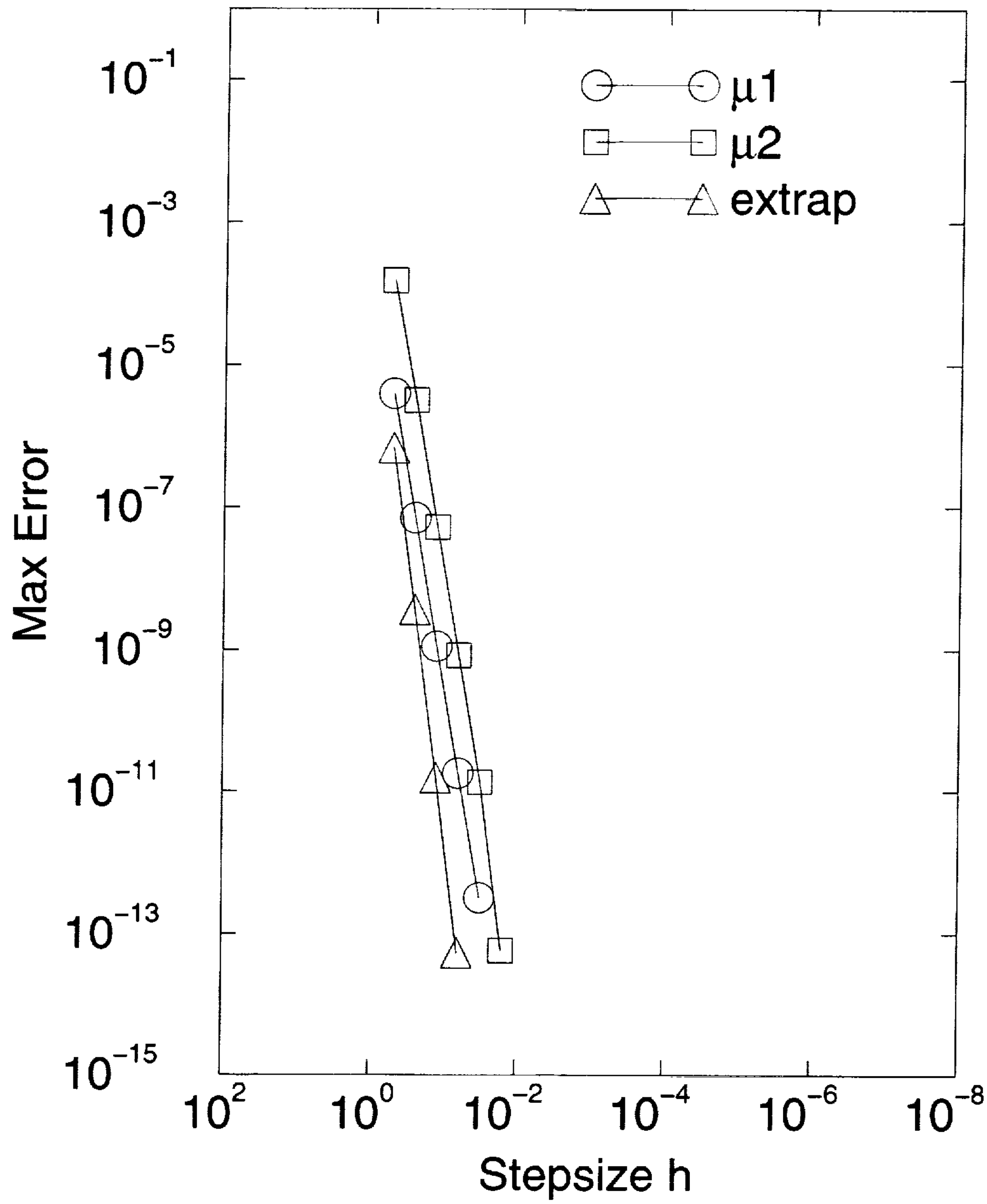

Figure 14.e Reduction of error for Problem 5 using a degree-4 Taylor series with $\mu_1 = \frac{1}{2} + i\frac{1}{2}\tan\frac{\pi}{10}$, $\mu_2 = \frac{1}{2} + i\frac{1}{2}\tan\frac{3\pi}{10}$, and with extrapolation.

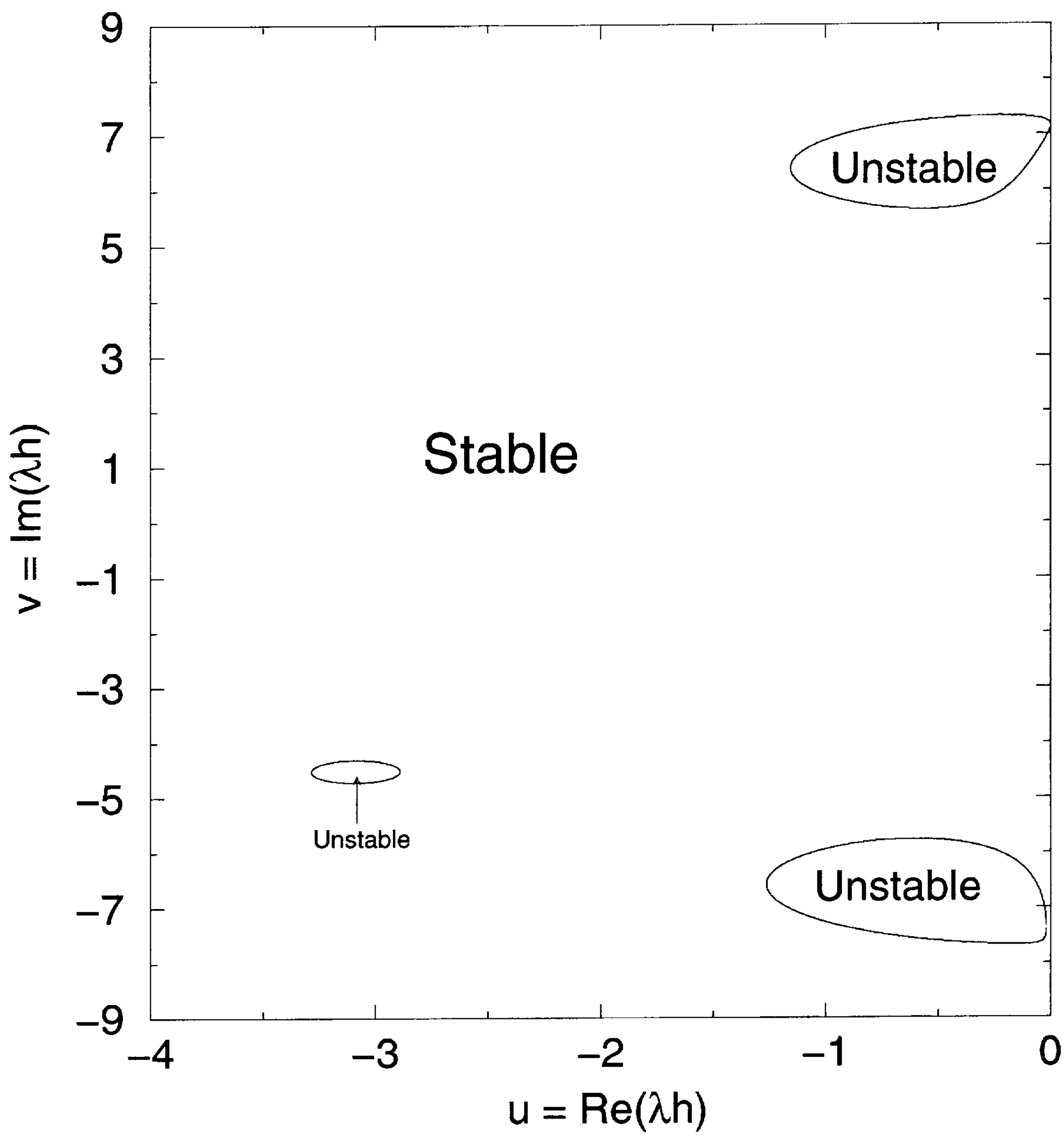

Figure 15.a Stability region for a degree-5 Taylor series with extrapolation.

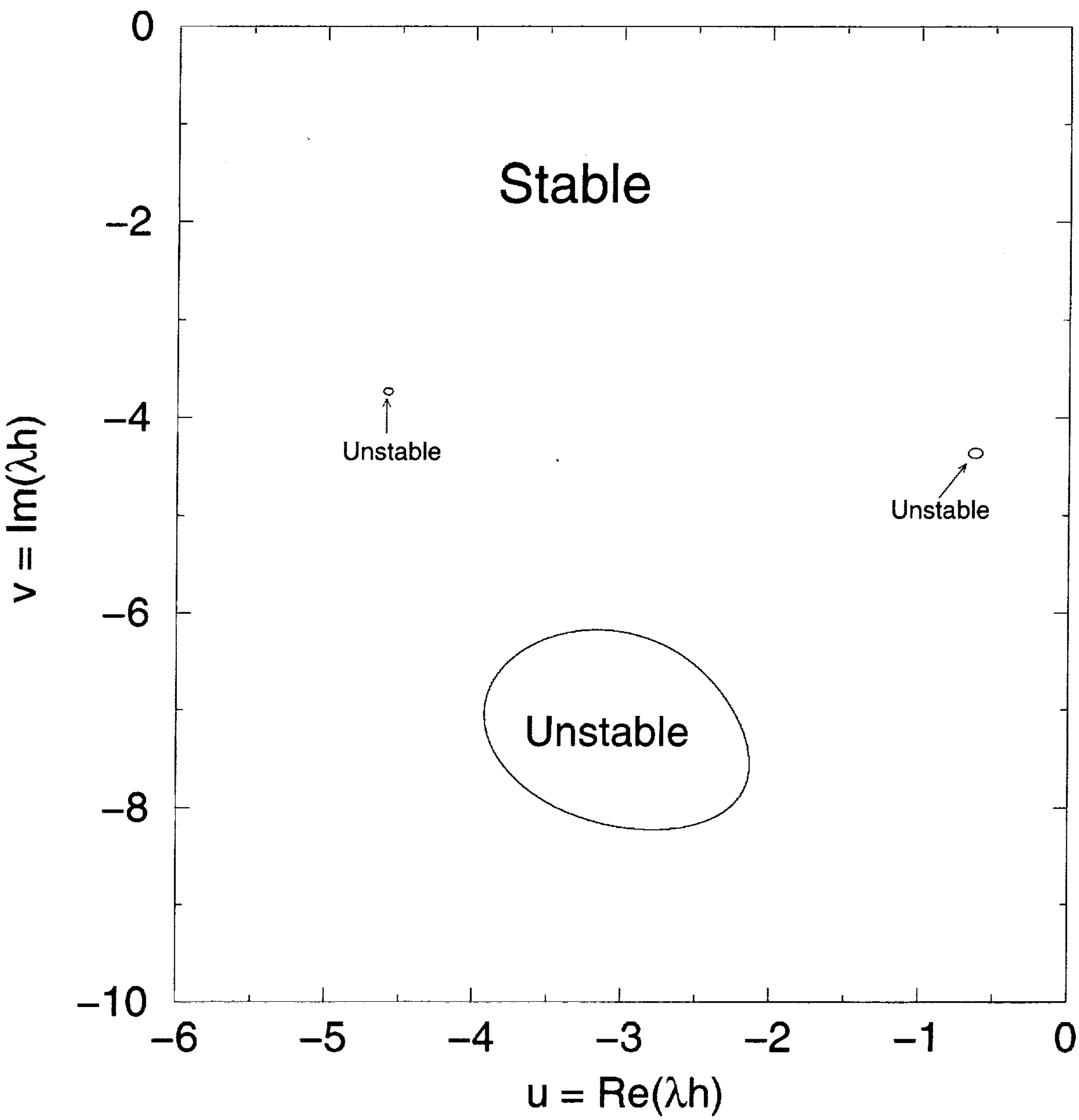

Figure 15.b Stability region for a degree-6 Taylor series with extrapolation.

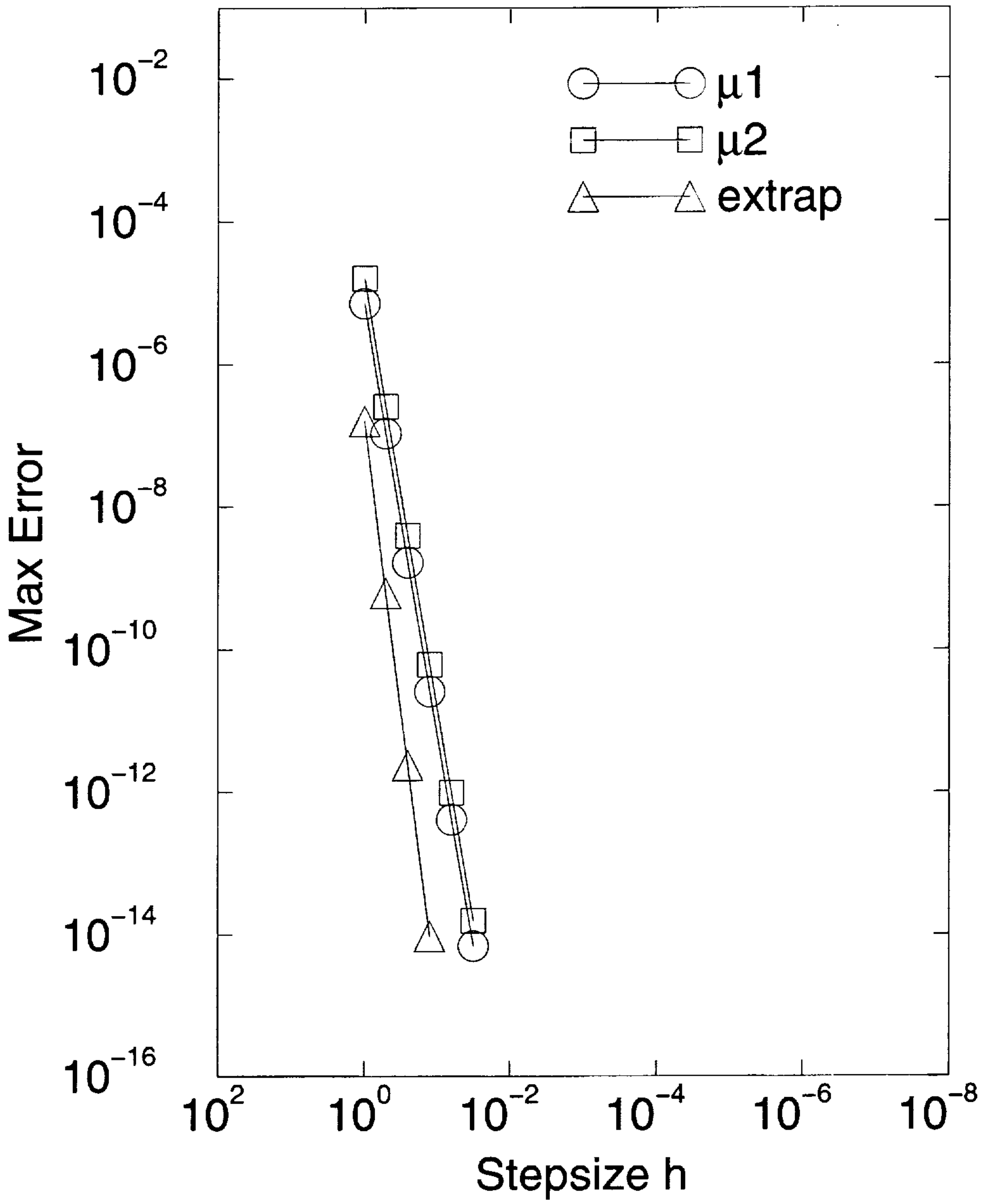

Figure 16.a Reduction of error for Problem 1 using a degree-5 Taylor series with $\mu_1 = \frac{1}{2}$, $\mu_2 = \frac{1}{2} + i\,\frac{1}{2}\tan\frac{\pi}{6}$, and with extrapolation.

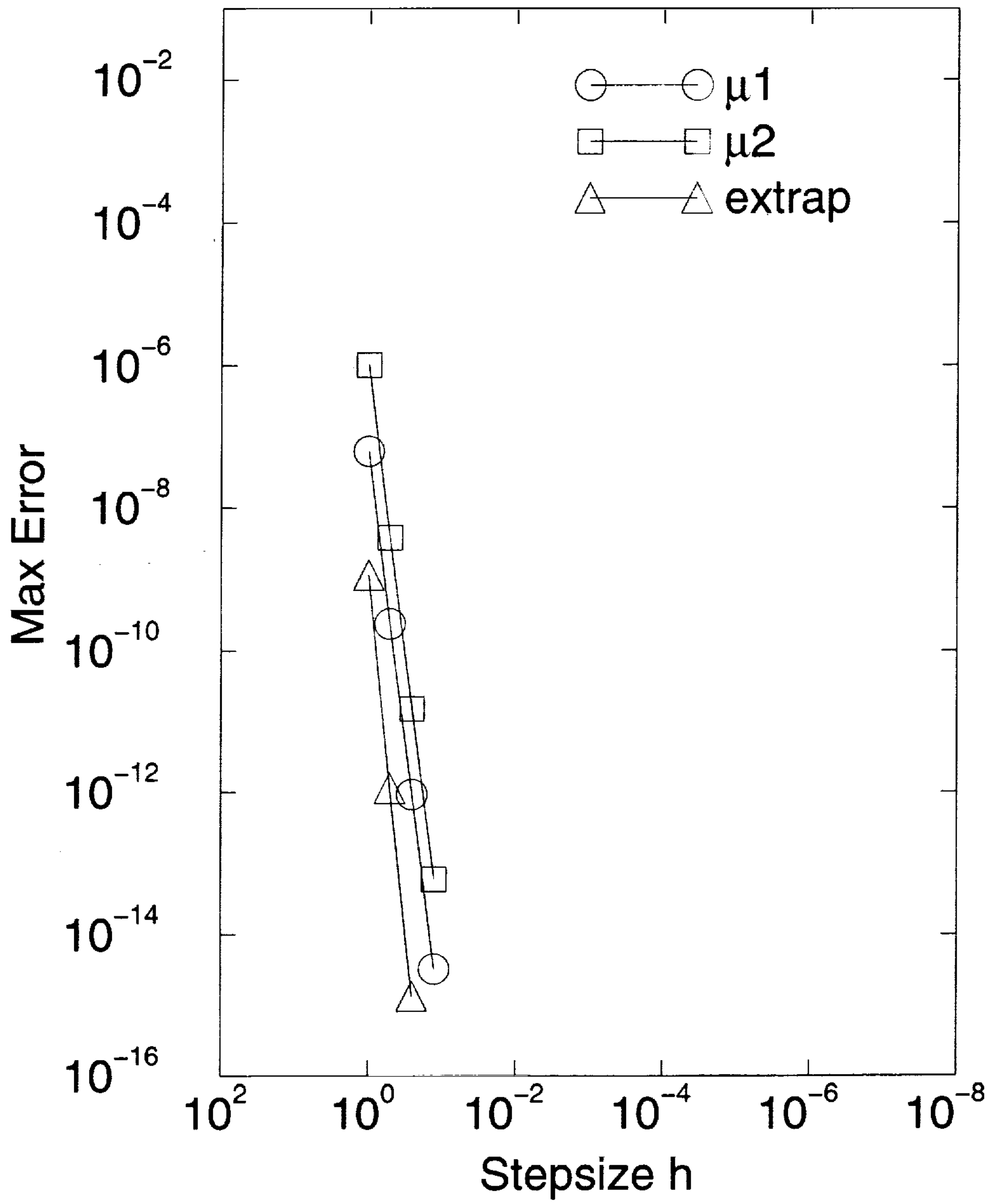

Figure 16.b Reduction of error for Problem 1 using a degree-6 Taylor series with $\mu_1 = \frac{1}{2} + i\,\frac{1}{2}\tan\frac{\pi}{14}$, $\mu_2 = \frac{1}{2} + i\,\frac{1}{2}\tan\frac{3\pi}{14}$, and with extrapolation.

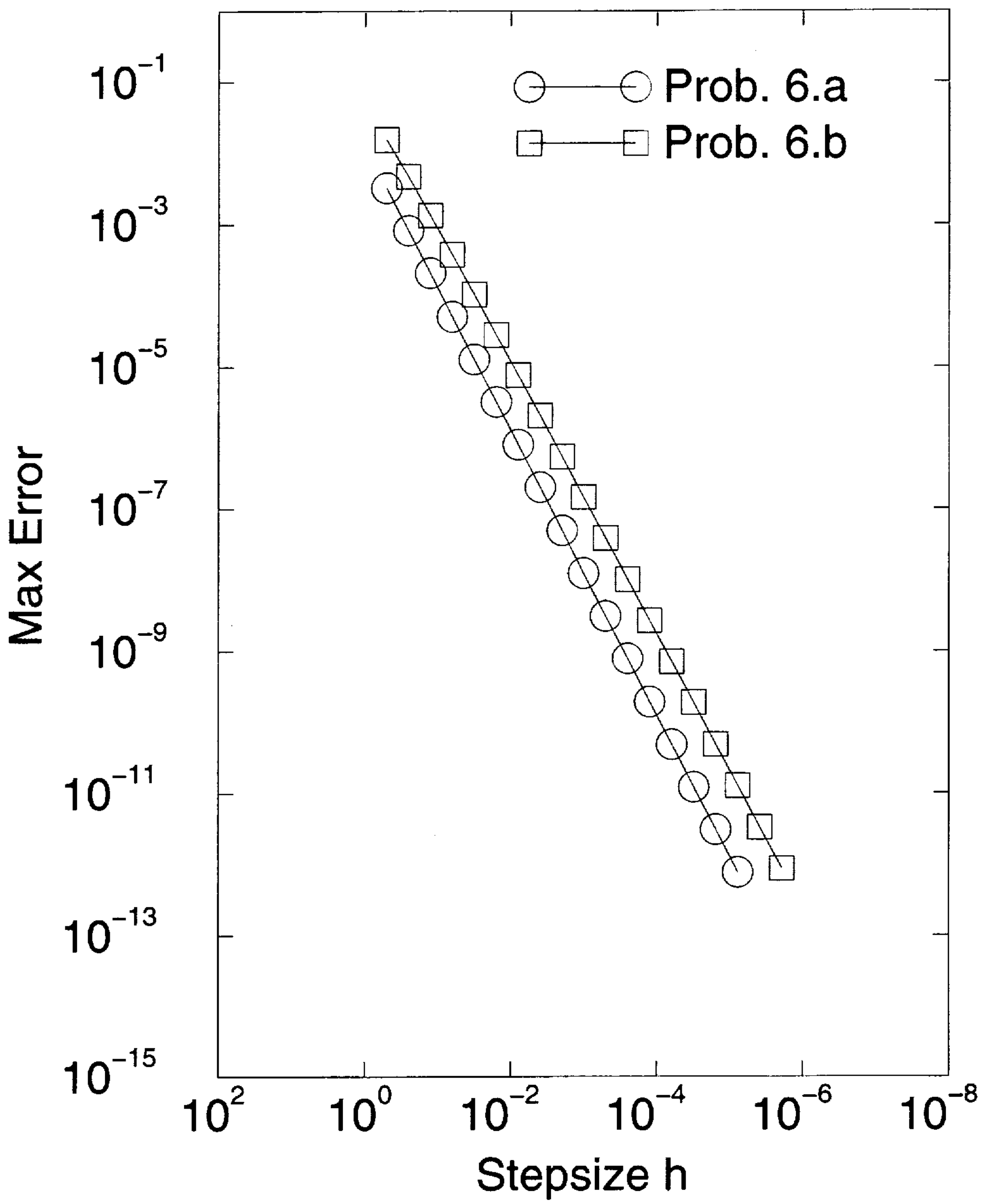

Figure 17.a Reduction of error for Problems 6.a,b using a degree-1 Taylor series with $\mu = \frac{1}{2}$.

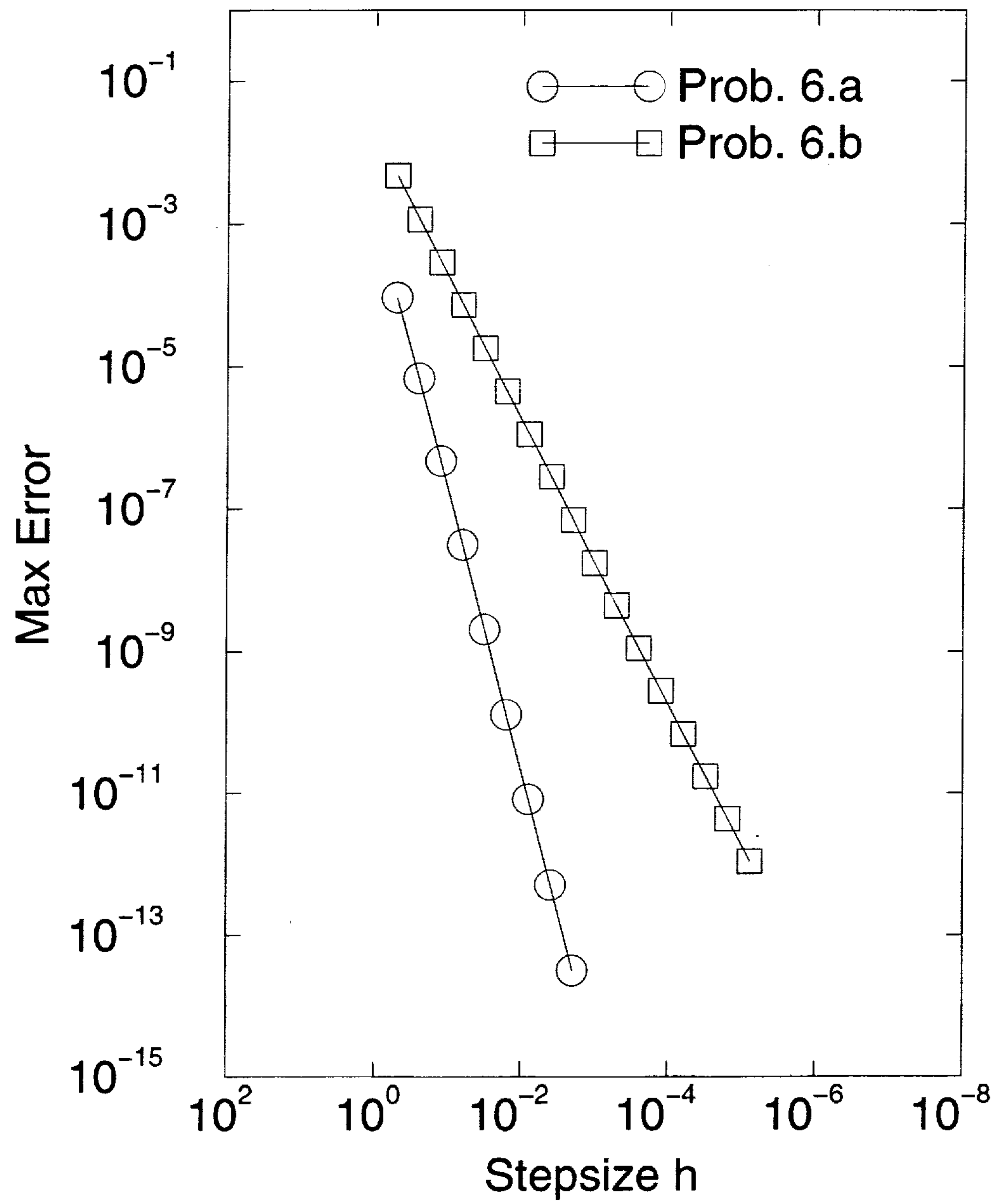

Figure 17.b Reduction of error for Problems 6.a,b using a degree-2 Taylor series with $\mu = \frac{1}{2} + i\frac{\sqrt{3}}{6}$.

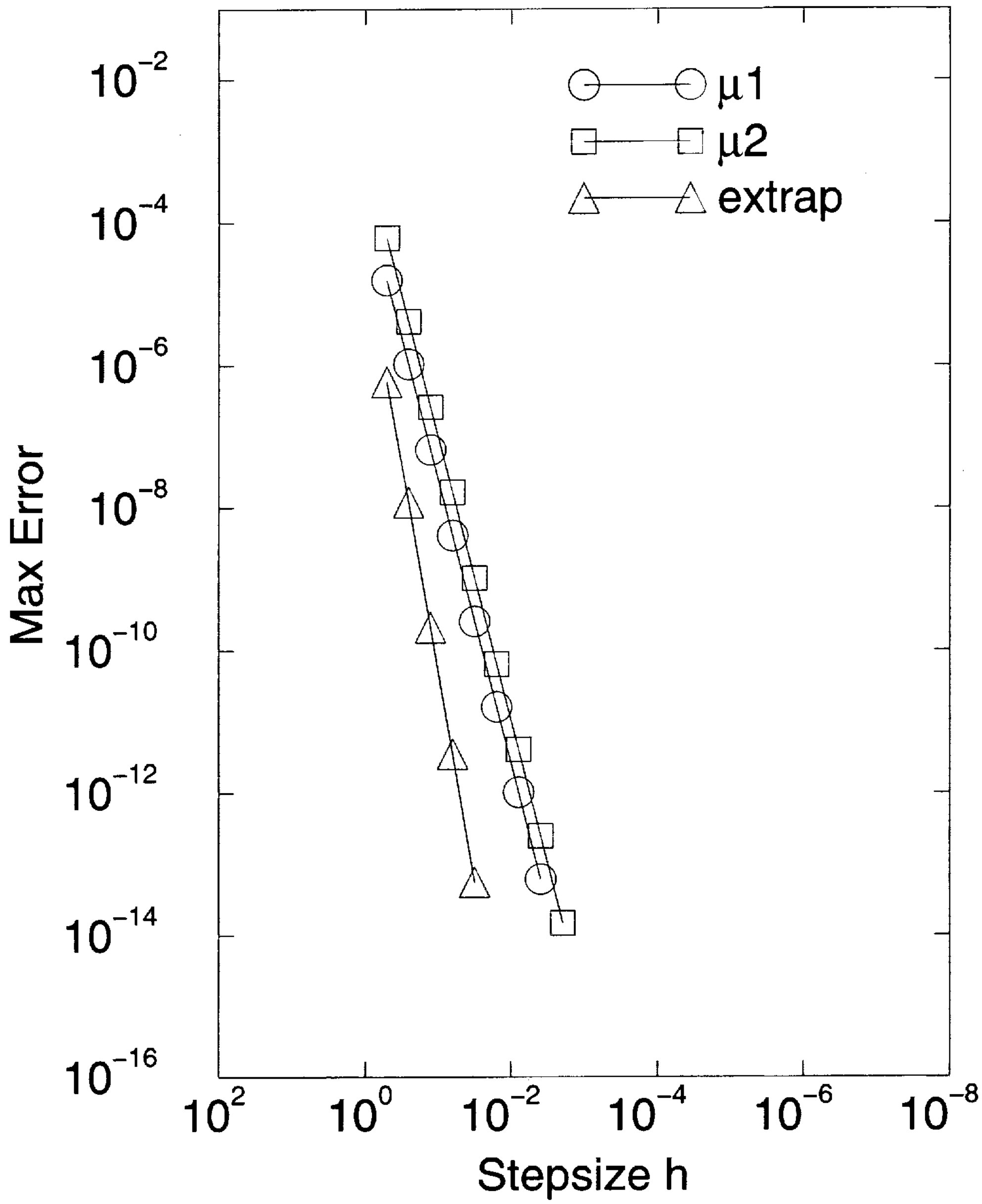

Figure 17.c Reduction of error for Problem 6.a using a degree-3 Taylor series with $\mu_1 = \frac{1}{2}$, $\mu_2 = \frac{1}{2} + i\,\frac{1}{2}$, and with extrapolation.

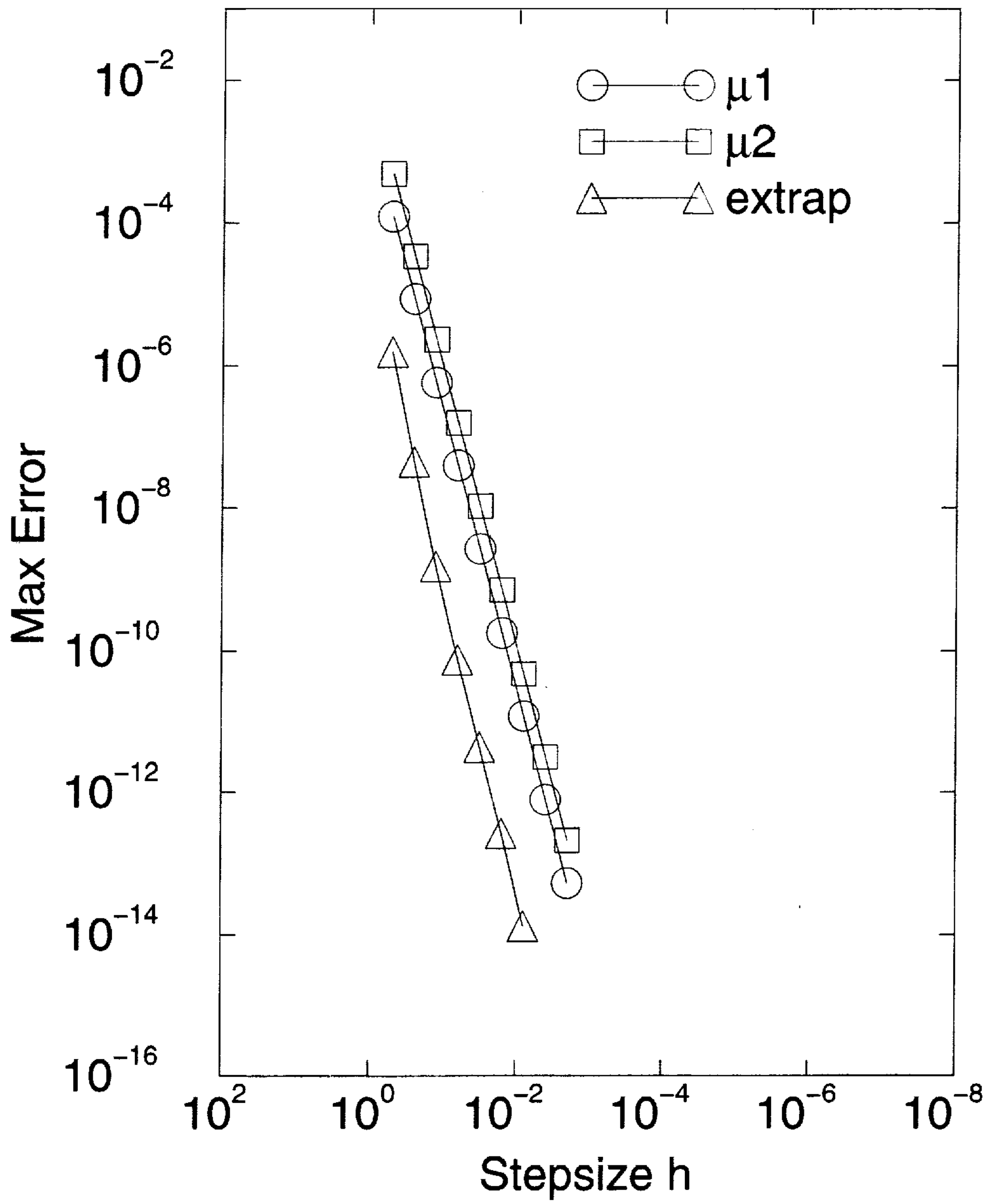

Figure 17.d Reduction of error for Problem 6.b using a degree-3 Taylor series with $\mu_1 = \frac{1}{2}$, $\mu_2 = \frac{1}{2} + i\,\frac{1}{2}$, and with extrapolation.

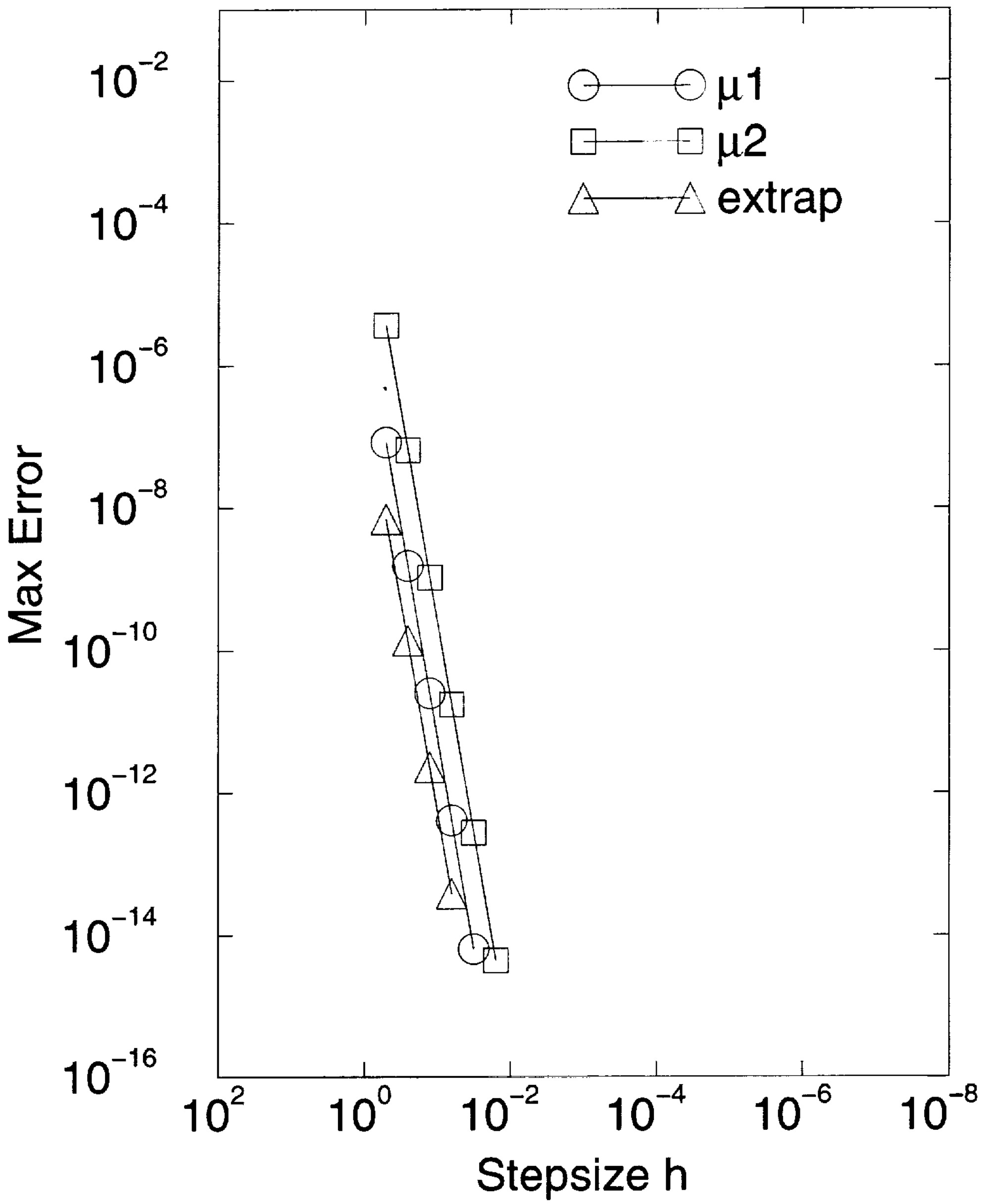

Figure 17.e Reduction of error for the Problem 6.a using a degree-4 Taylor series with $\mu_1 = \frac{1}{2} + i\,\frac{1}{2}\,\tan\frac{\pi}{10}$, $\mu_2 = \frac{1}{2} + i\,\frac{1}{2}\,\tan\frac{3\pi}{10}$, and with extrapolation.

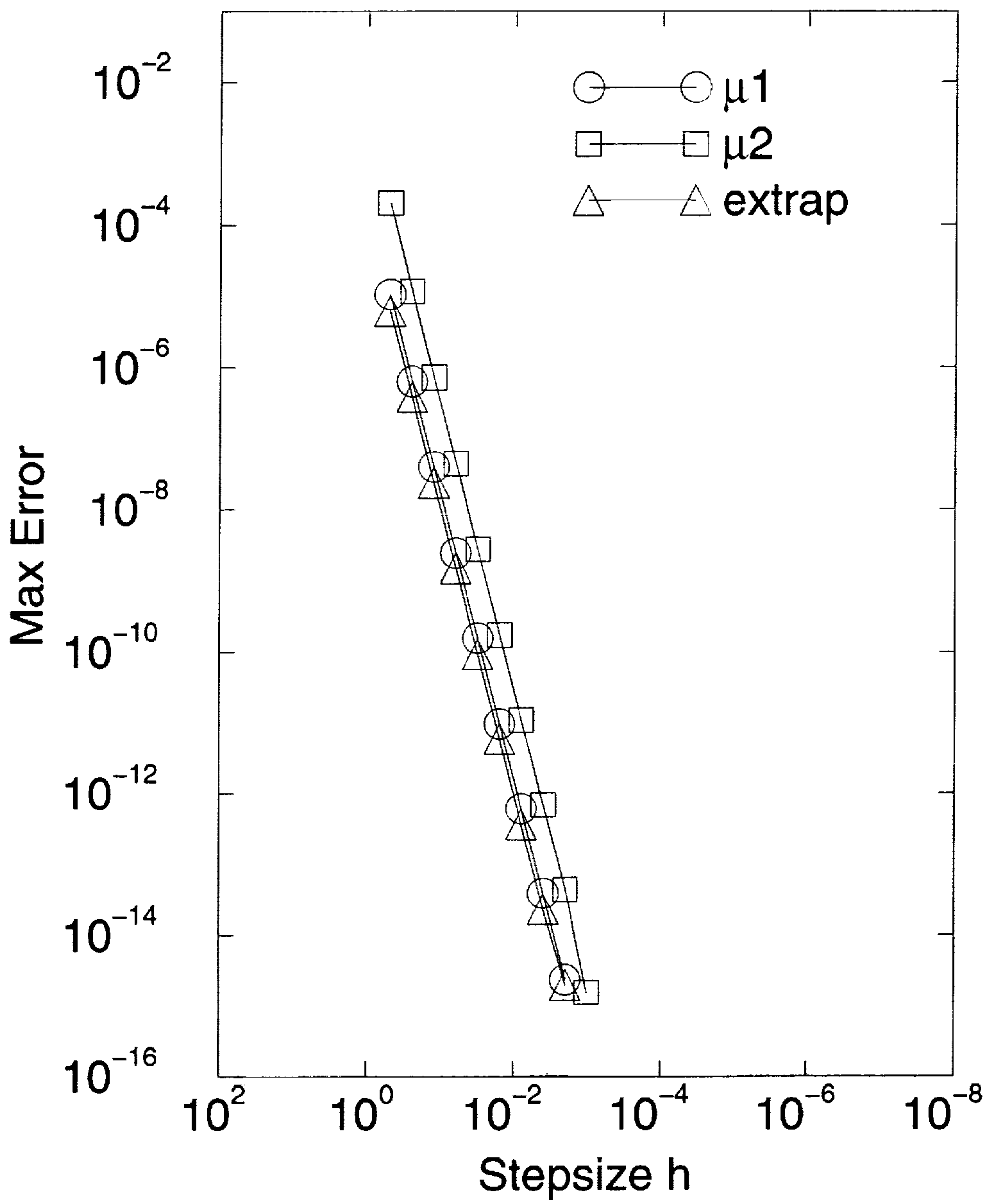

Figure 17.f Reduction of error for Problem 6.b using a degree-4 Taylor series with $\mu_1 = \frac{1}{2} + i\frac{1}{2}\tan\frac{\pi}{10}$, $\mu_2 = \frac{1}{2} + i\frac{1}{2}\tan\frac{3\pi}{10}$, and with extrapolation.

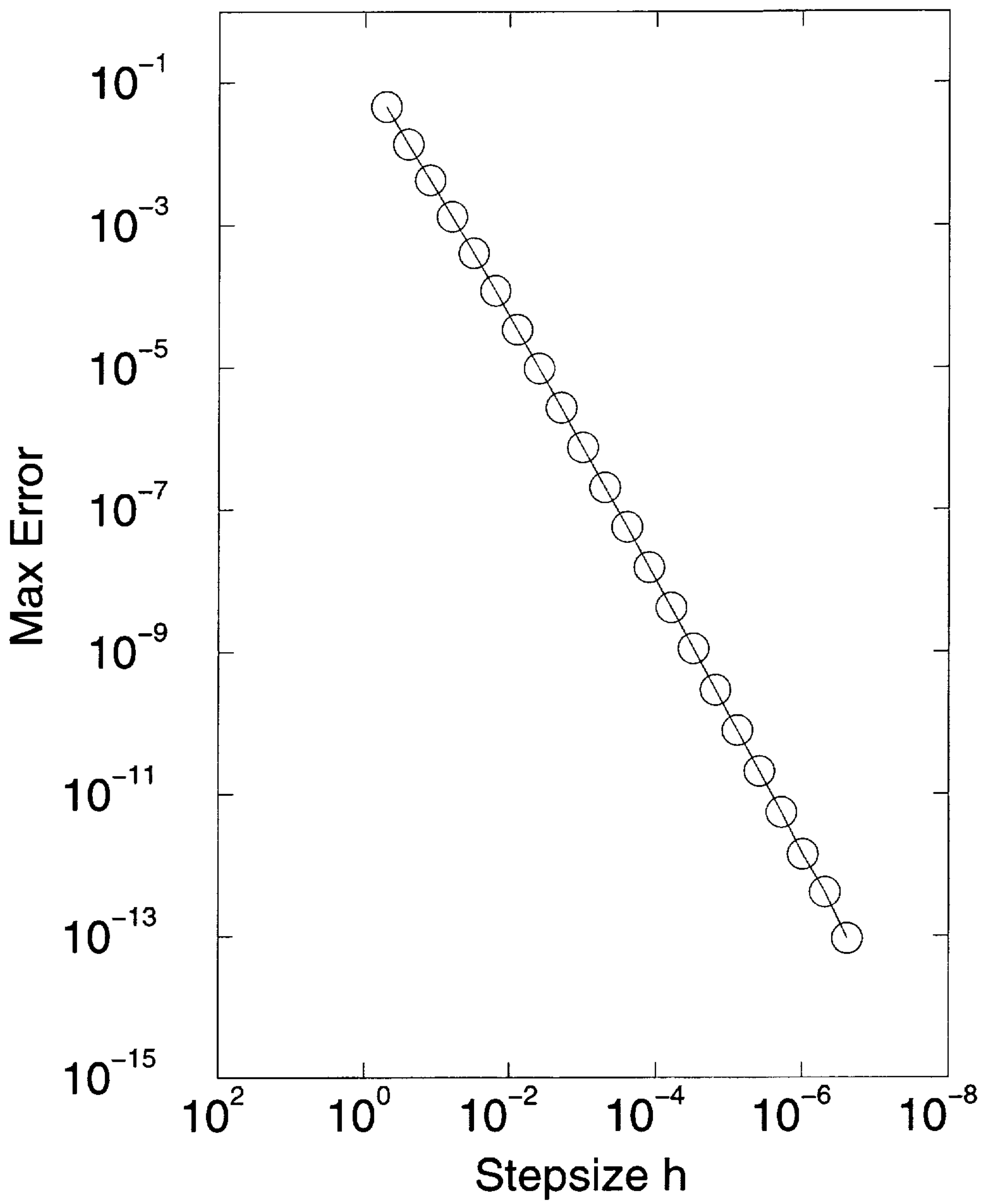

Figure 18.a   Reduction of error for Problem 7 using a degree-1 Taylor series with $\mu = \frac{1}{2}$.

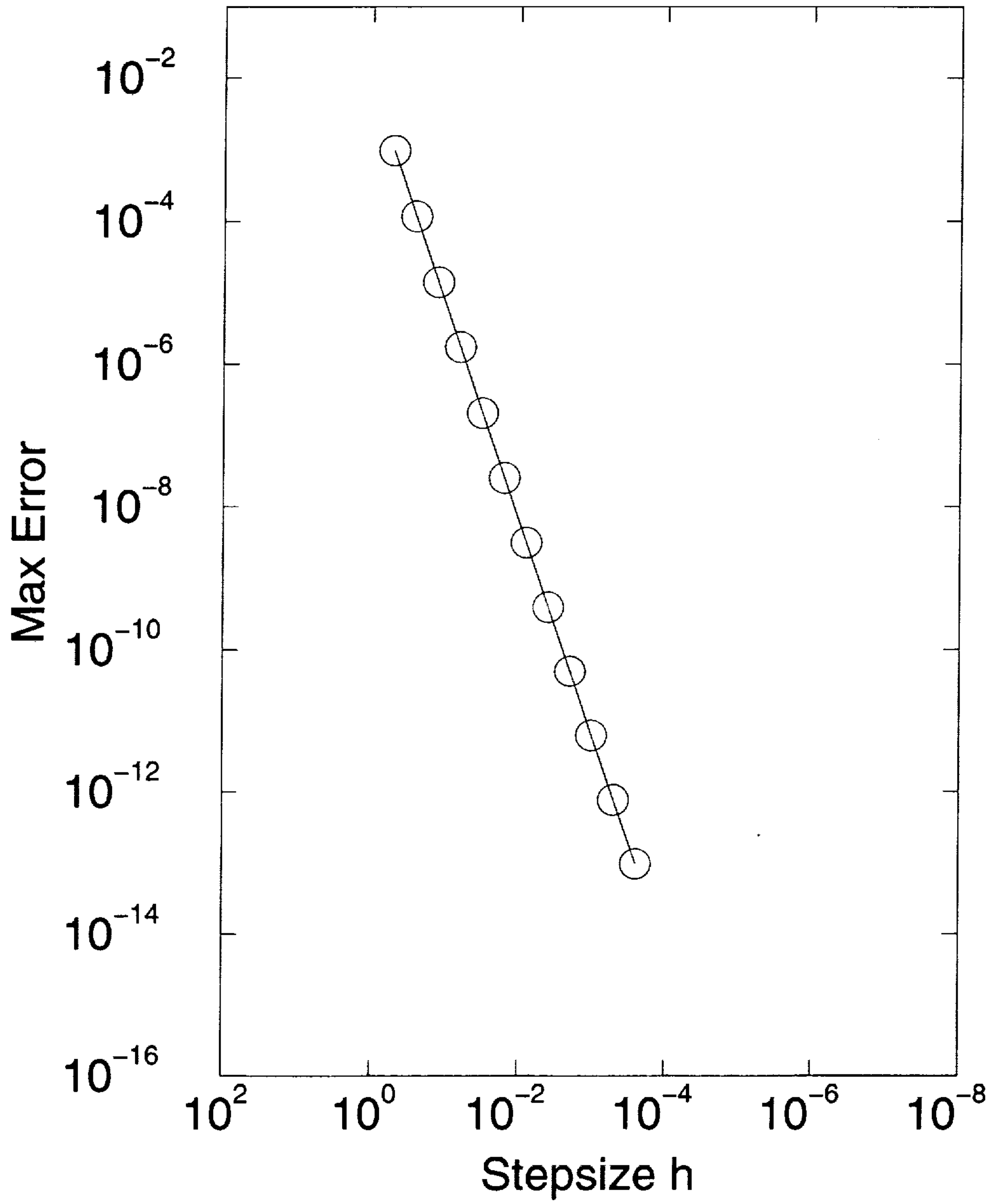

Figure 18.b Reduction of error for Problem 7 using a degree-2 Taylor series with $\mu = \frac{1}{2} + i\frac{\sqrt{3}}{6}$.

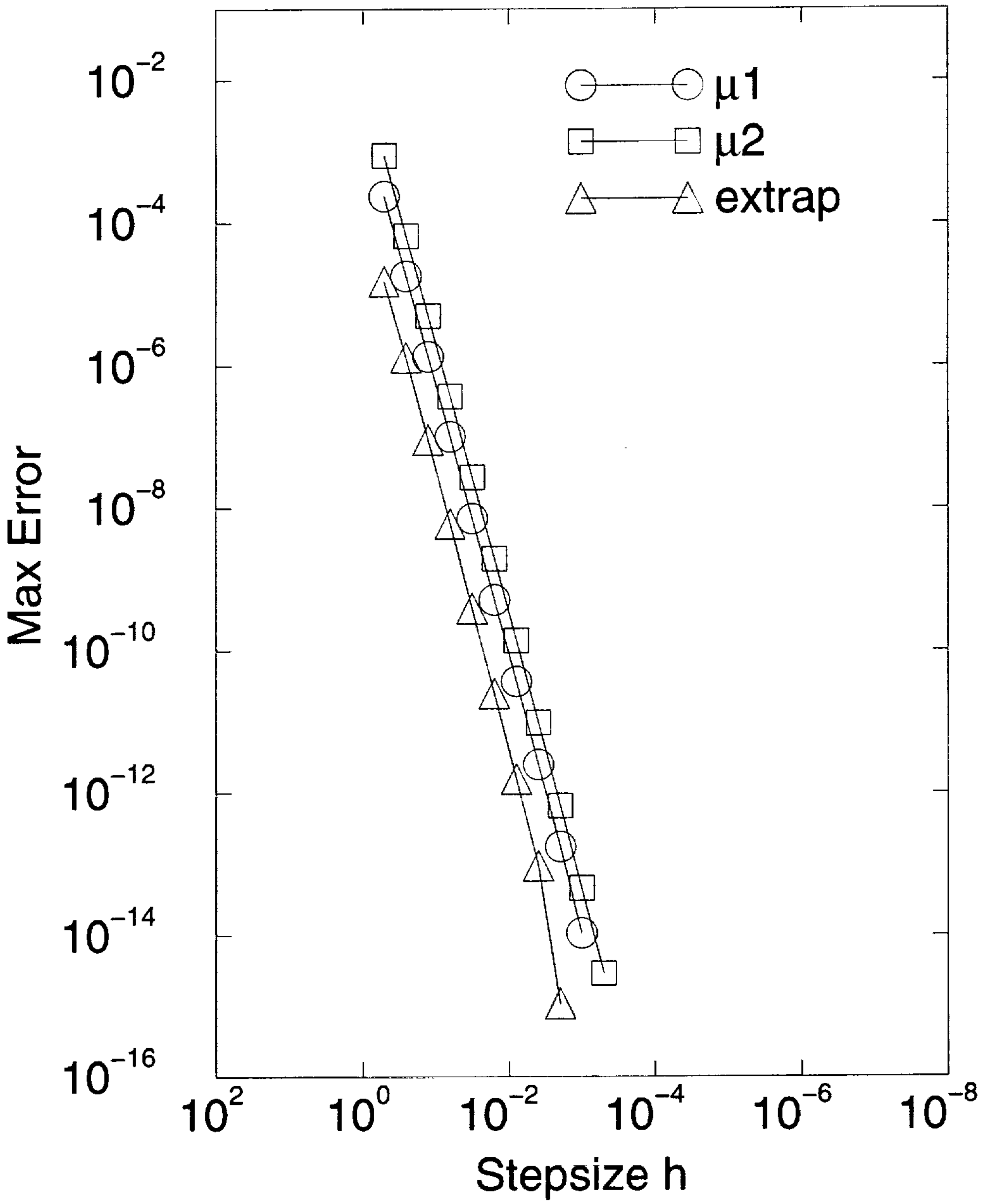

Figure 18.c Reduction of error for Problem 7 using a degree-3 Taylor series with $\mu_1 = \frac{1}{2}$, $\mu_2 = \frac{1}{2} + i\,\frac{1}{2}$, and with extrapolation.

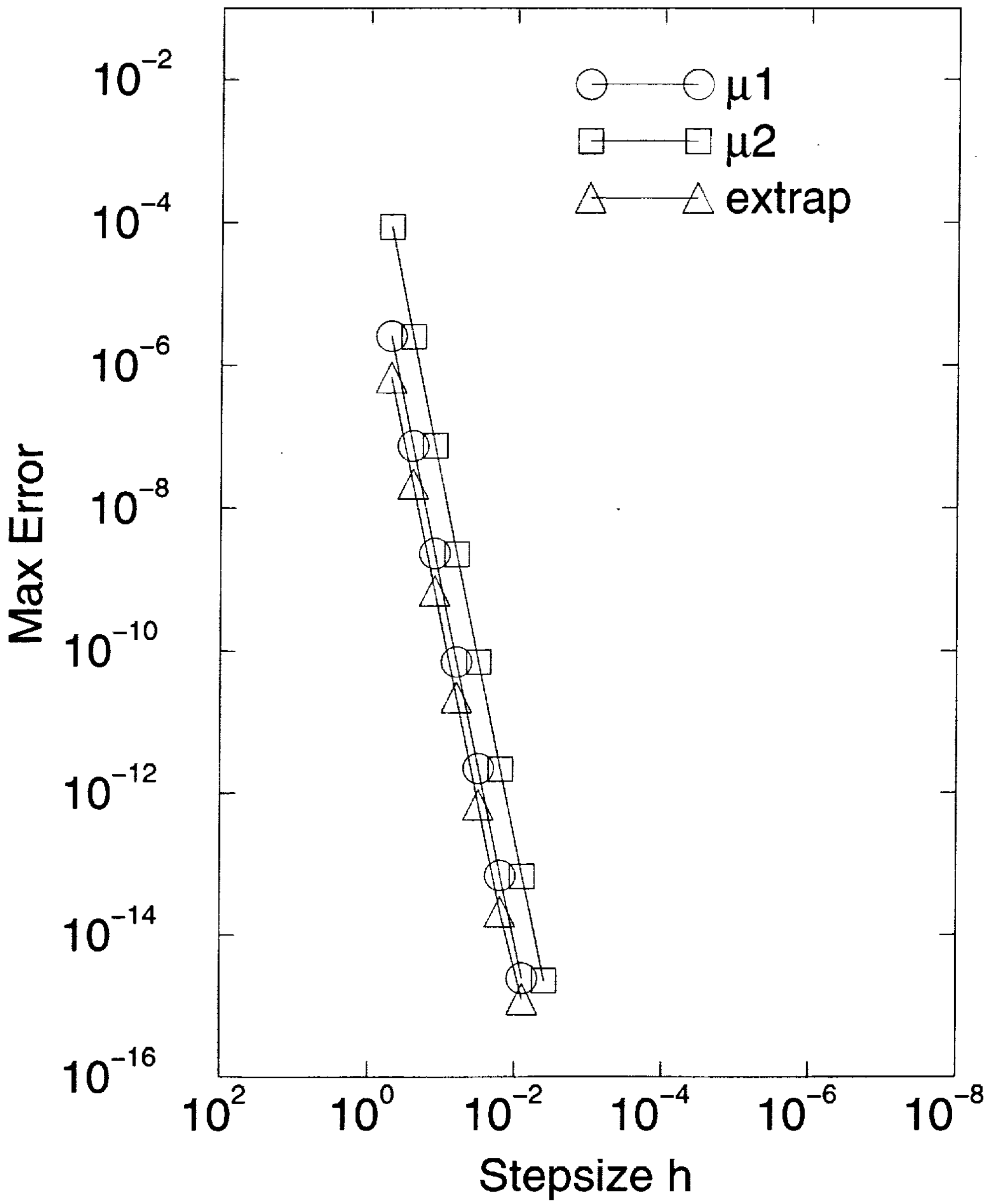

Figure 18.d Reduction of error for Problem 7 using a degree-4 Taylor series with $\mu_1 = \frac{1}{2} + i\,\frac{1}{2}\tan\frac{\pi}{10}$, $\mu_2 = \frac{1}{2} + i\,\frac{1}{2}\tan\frac{3\pi}{10}$, and with extrapolation.

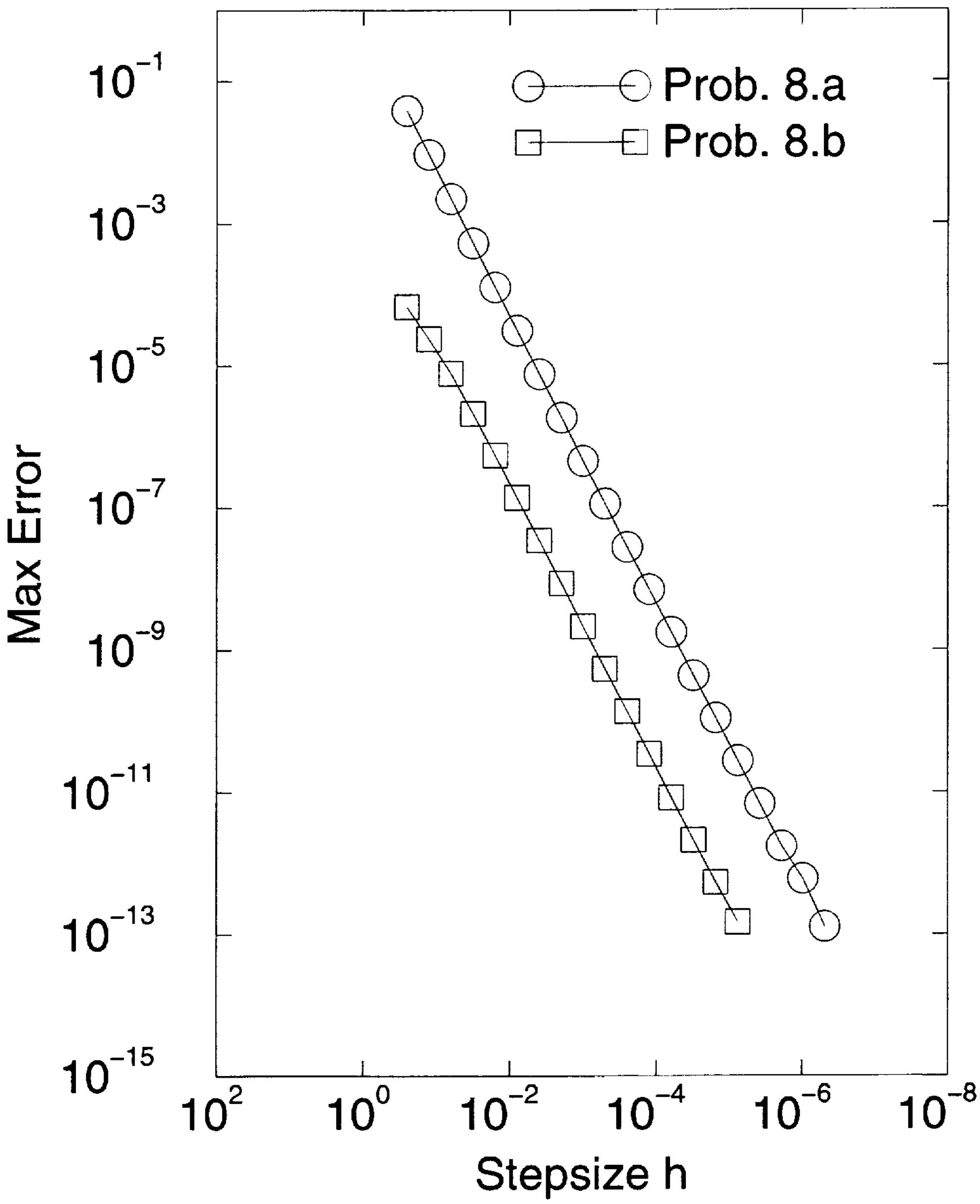

Figure 19.a Reduction of error for Problems 8.a,b using a degree-1 Taylor series with $\mu = \frac{1}{2}$.

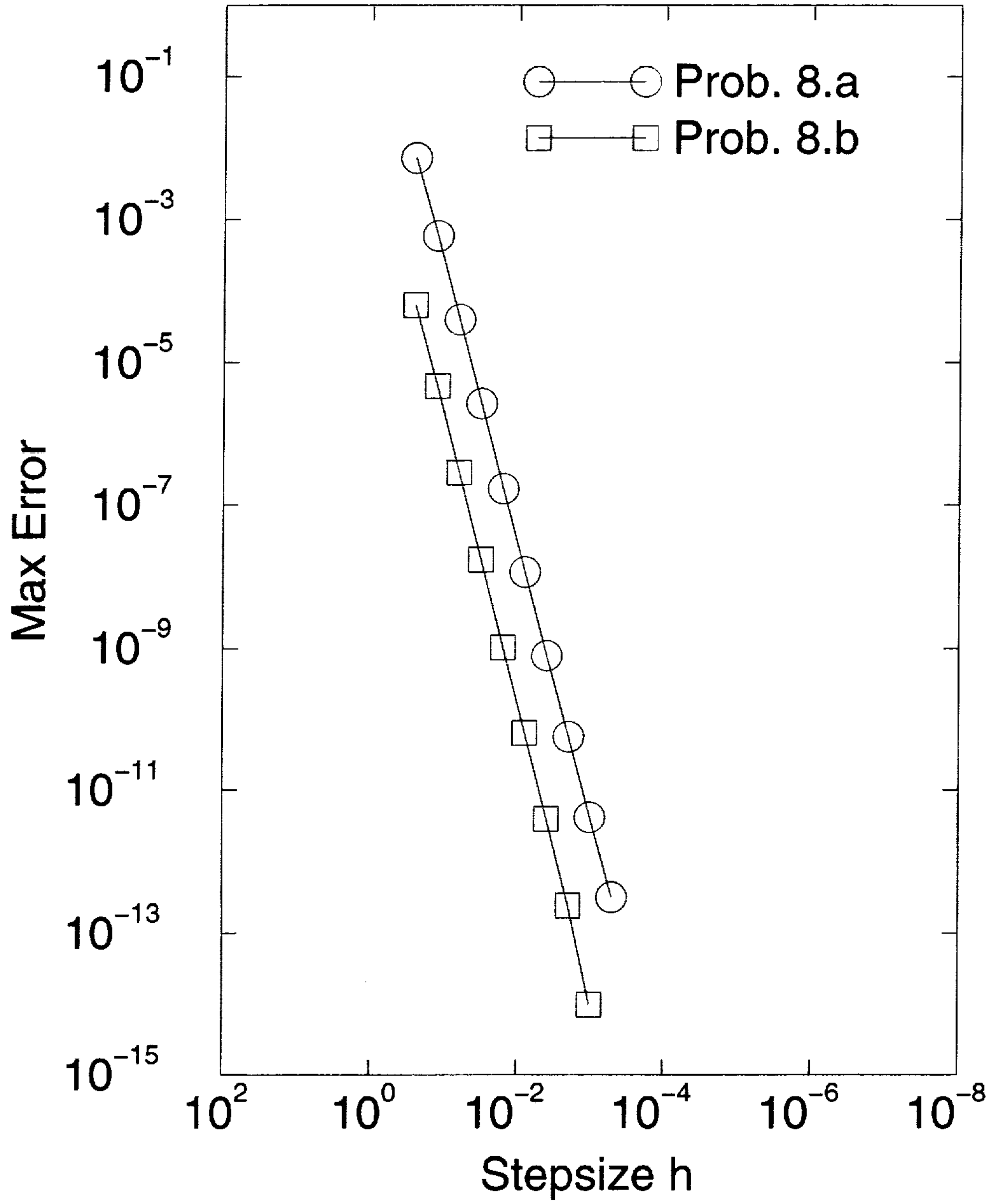

Figure 19.b Reduction of error for Problems 8.a,b using a degree-2 Taylor series with $\mu = \frac{1}{2} + i\frac{\sqrt{3}}{6}$.

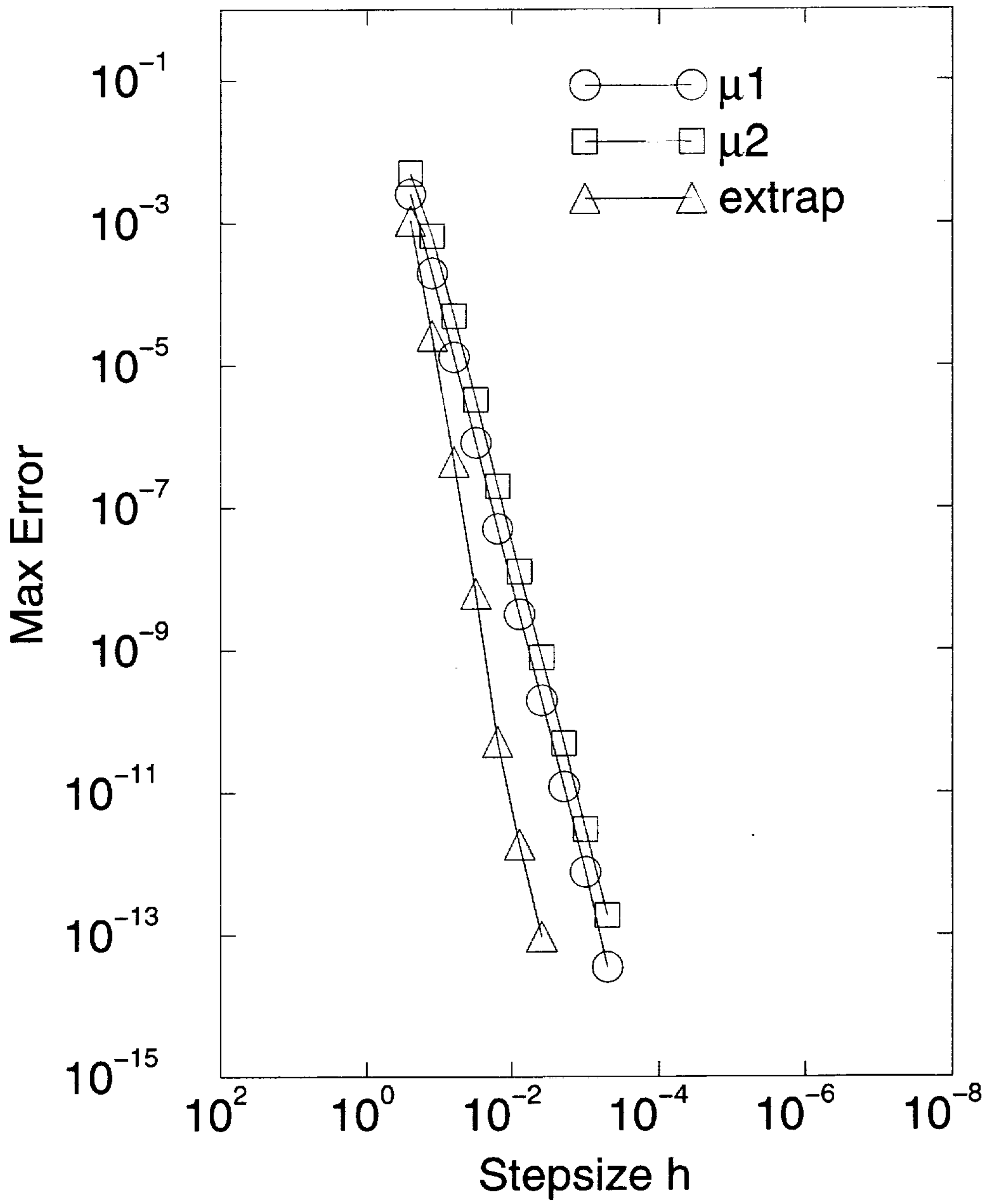

Figure 19.c Reduction of error for Problem 8.a using a degree-3 Taylor series with $\mu_1 = \frac{1}{2}$, $\mu_2 = \frac{1}{2} + i\,\frac{1}{2}$, and with extrapolation.

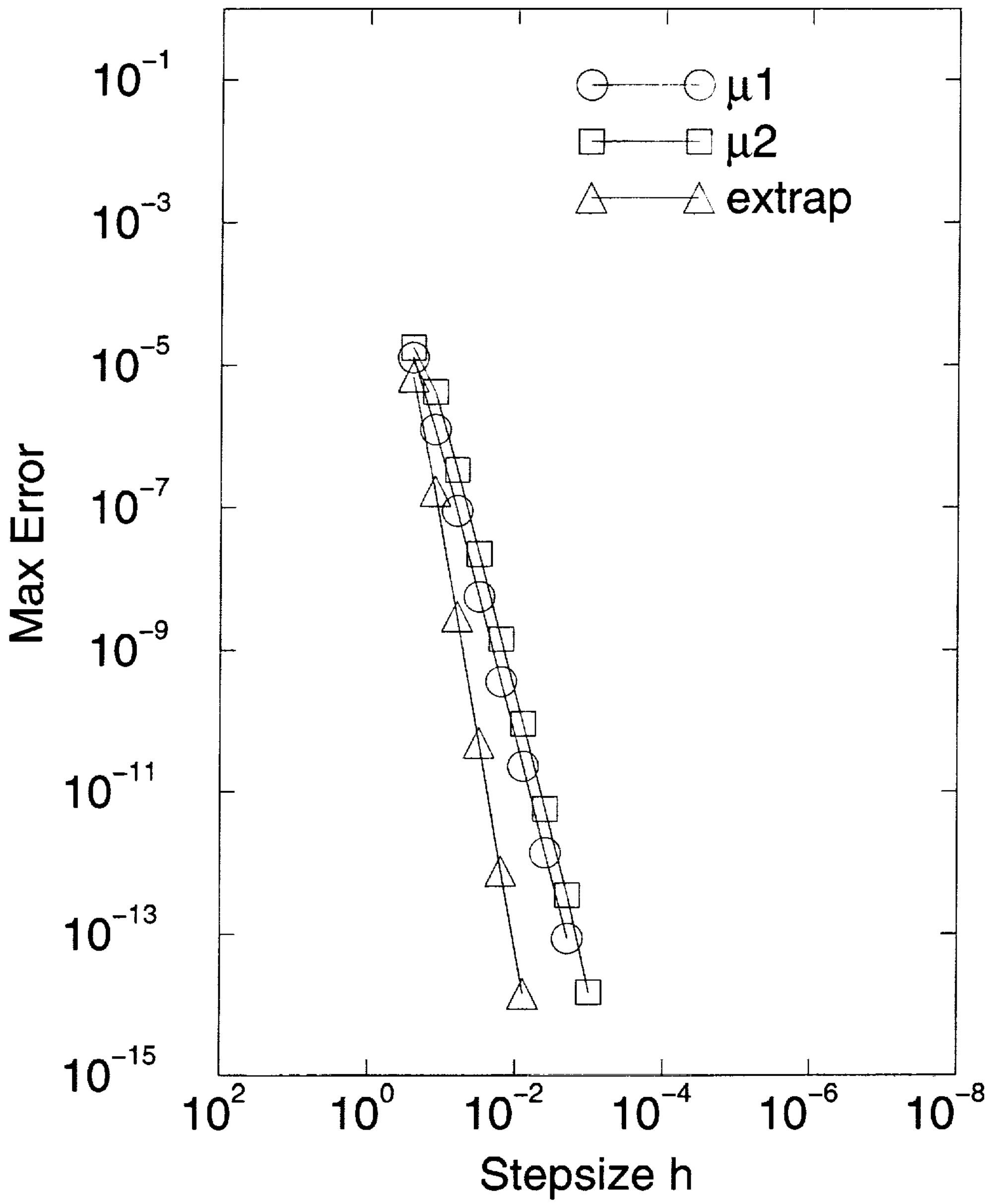

Figure 19.d Reduction of error for Problem 8.b using a degree-3 Taylor series with $\mu_1 = \frac{1}{2}$, $\mu_2 = \frac{1}{2} + i\,\frac{1}{2}$, and with extrapolation.

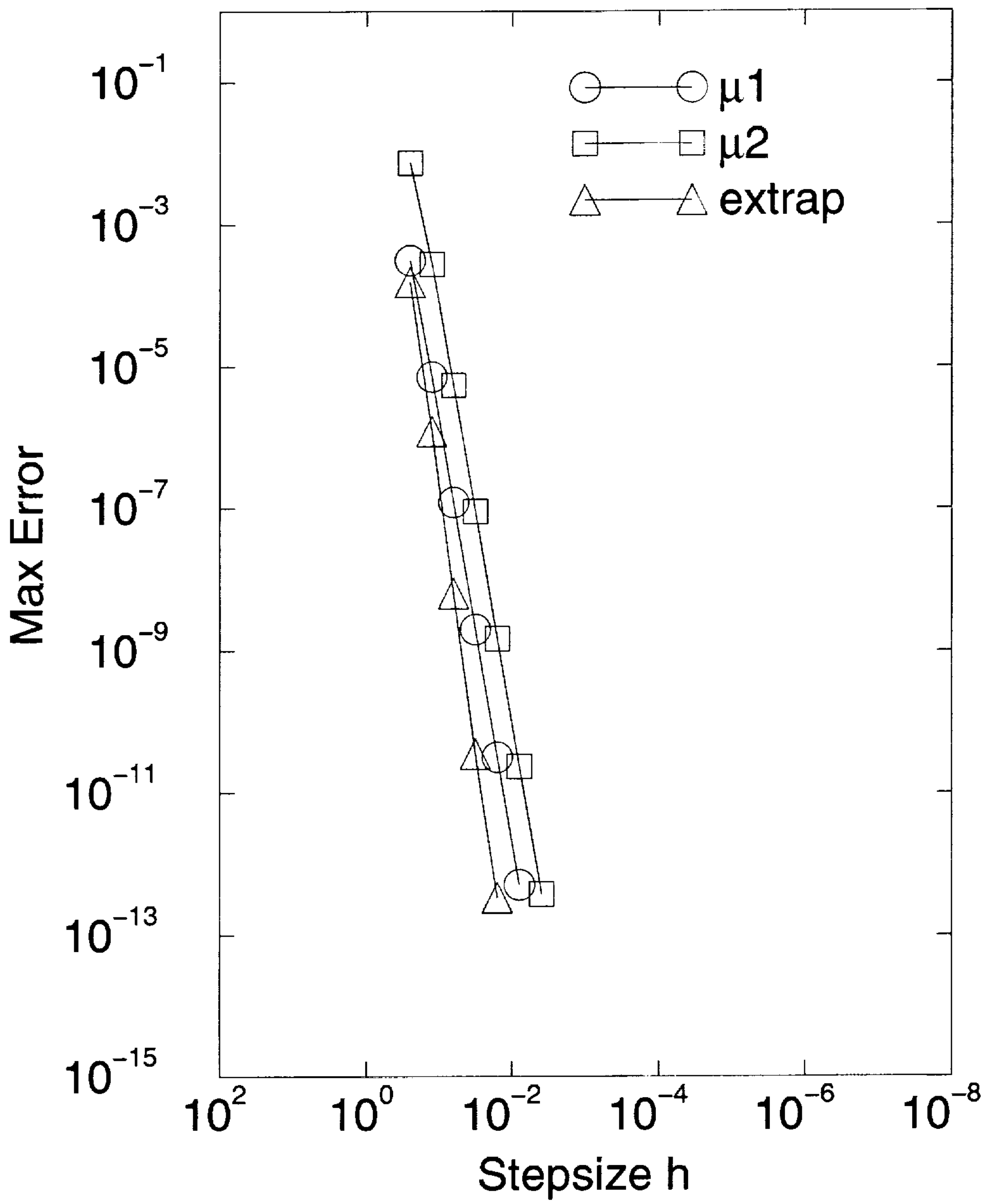

Figure 19.e Reduction of error for Problem 8.a using a degree-4 Taylor series with $\mu_1 = \frac{1}{2} + i\frac{1}{2}\tan\frac{\pi}{10}$, $\mu_2 = \frac{1}{2} + i\frac{1}{2}\tan\frac{3\pi}{10}$, and with extrapolation.

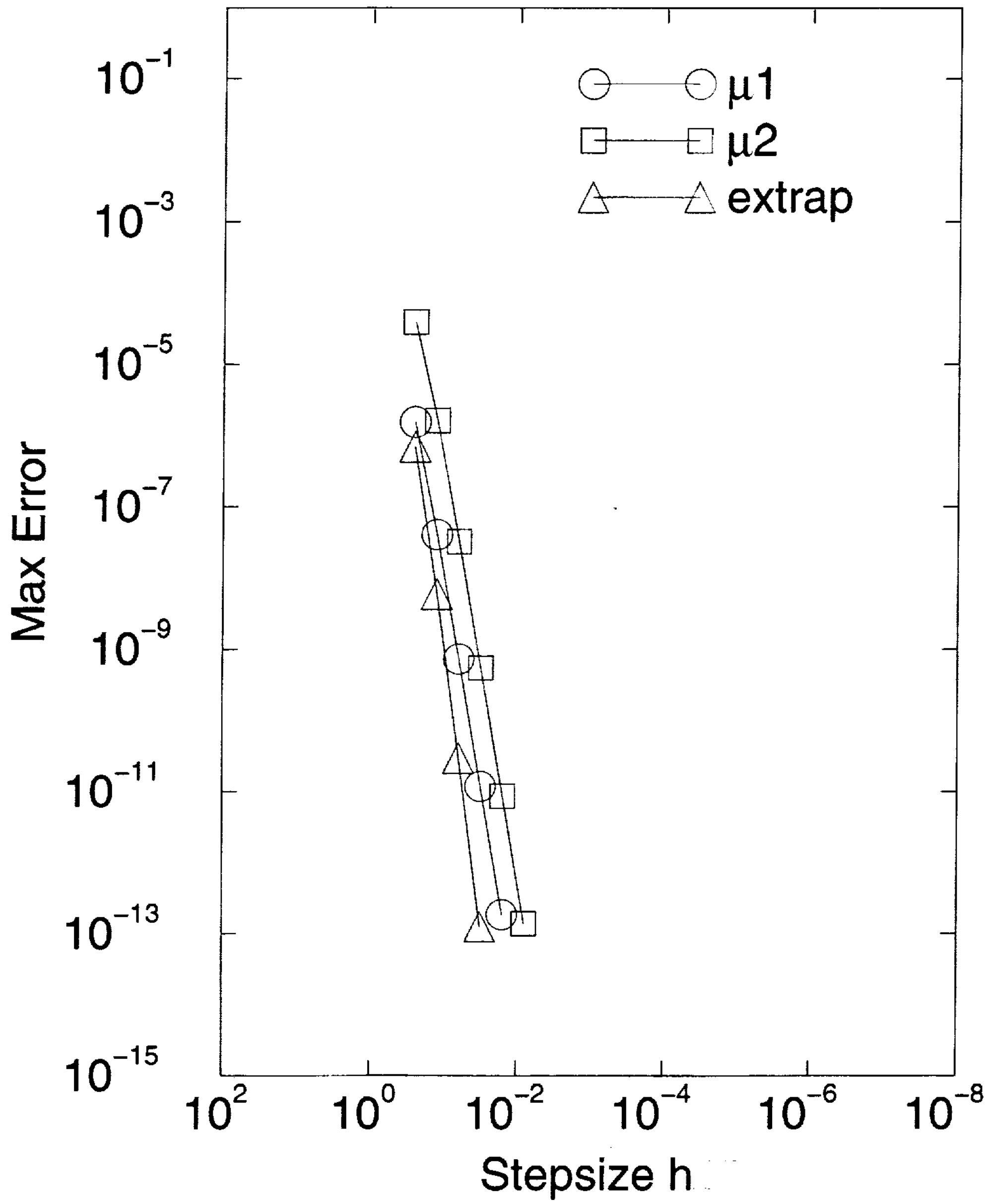

Figure 19.f Reduction of error for Problem 8.b using a degree-4 Taylor series with $\mu_1 = \frac{1}{2} + i\frac{1}{2}\tan\frac{\pi}{14}$, $\mu_2 = \frac{1}{2} + i\frac{1}{2}\tan\frac{3\pi}{14}$, and with extrapolation.

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13. ABSTRACT *(Maximum 200 words)*

In this paper we introduce a new class of numerical methods for integrating ODE initial value problems. Specifically, we propose an extension of the Taylor series method which significantly improves its accuracy and stability while also increasing its range of applicability. To advance the solution from t_n to t_{n+1}, we expand a series about the intermediate point $t_{n+\mu} := t_n + \mu h$, where h is the stepsize and μ is an arbitrary parameter called an expansion coefficient. We show that, in general, a Taylor series of degree k has exactly k expansion coefficients which raise its order of accuracy. The accuracy is raised by one order if k is odd, and by two orders if k is even. In addition, if k is three or greater, local extrapolation can be used to raise the accuracy two additional orders. We also examine stability for the problem $y' = \lambda y$, Re $(\lambda) < 0$, and identify several A-stable schemes. Numerical results are presented for both fixed and variable stepsizes. It is shown that implicit Taylor series methods provide an effective integration tool for most problems, including stiff systems and ODE's with a singular point.

14. SUBJECT TERMS

Taylor series; Implicit, Ordinary differential equation; ODE; Initial value problem; Time marching; Numerical integration; Systems of equations; Stiff equations; Singular initial value problem

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