MATHEMATICS OF COMPUTATION, VOLUME 32, NUMBER 143
JULY 1978, PAGES 751–762

On de Vogelaere's Method for $y'' = f(x, y)$

By John P. Coleman and Julie Mohamed

Abstract. Easily calculated truncation-error estimates are given which permit efficient automatic error control in computations based on de Vogelaere's method. An upper bound for the local truncation error is established, the interval of absolute stability is found to be $[-2, 0]$, and it is shown that the global truncation error is of order h^4 where h is the steplength.

1. Introduction. Ordinary differential equations of the special form

$$y'' = f(x, y), \tag{1}$$

and systems of such equations, arise in a variety of physical contexts. Examples include atomic and nuclear scattering problems, molecular-dynamics calculations for liquids and gases, and stellar mechanics. A numerical method proposed by de Vogelaere [3] has been used extensively to solve equations of this type (e.g. [1], [8], [9] and [12]), and Chandra [2] has published a computer program which uses de Vogelaere's method to solve the differential equations arising in a close-coupling formulation of quantum mechanical scattering problems. Chandra's program makes no attempt to monitor the local truncation error, and leaves the choice of steplength strategy entirely to the user.

A major objective in recent work on numerical methods for nonstiff ordinary differential equations of first order has been the development of efficient codes which automatically select steps as large as possible while satisfying some error criterion specified by the user (see surveys by Shampine et al. [11] and by Lambert [7]). Adopting this philosophy, our aim has been to improve on existing implementations of de Vogelaere's method for the second-order equation (1) by incorporating a method of truncation-error estimation, and an automatic mesh-selection facility.

For ease of reference, and to establish notation, we present in Section 2 a derivation of de Vogelaere's method based on Taylor expansions. The estimation of the local truncation error, on which the choice of steplength depends, is discussed in Section 3. Despite the frequent use of de Vogelaere's method we are unaware of any previous error analysis, or any study of the stability of the method; later sections of the paper deal with these matters. A bound for the local truncation error is derived in Section 4, the stability region of the method is established in Section 5, and the global truncation error is examined in Section 6.

2. Derivation of de Vogelaere's Method. The differential equation (1) is to be solved, in some real interval $[a, b]$, subject to the initial conditions

Received August 4, 1977.
AMS (MOS) subject classifications (1970). Primary 65L05; Secondary 81.65.

$$y(x_0) = y_0, \qquad z(x_0) = z_0,$$

where y_0 and z_0 are specified numbers and

$$z(x) = \frac{dy}{dx}.$$

The mesh points, which in general are not evenly spaced, are denoted by x_n ($n = 0, 1, \ldots$), y_n is an approximation to the exact solution $y(x_n)$ at the mesh point x_n, and we shall also use the abbreviation

$$f_n = f(x_n, y_n).$$

Let h be the initial steplength, so that

$$x_1 = x_0 + h, \qquad x_2 = x_0 + 2h.$$

Then, by using the equations

$$hf_0' = f_0 - f_{-1} + \frac{h^2}{2} f_0'' + O(h^3)$$

and

$$hf_0' + \frac{h^2}{2} f_0'' = f_1 - f_0 - \frac{h^3}{6} f_0''' + O(h^4)$$

in Taylor expansions about x_0, we obtain

$$y(x_1) = y_0 + hz_0 + \frac{h^2}{6}(4f_0 - f_{-1}) + \frac{h^4}{8} f_0'' + O(h^5) \tag{2}$$

and

$$y(x_2) = y_0 + 2hz_0 + \frac{h^2}{3}(4f_1 + 2f_0) + \frac{2h^5}{45} f_0''' + O(h^6). \tag{3}$$

These expressions are valid provided that any errors in f_{-1} and f_1 are of order h^3 and h^4, respectively.

The de Vogelaere algorithm is obtained by neglecting $O(h^4)$ terms in (2) and $O(h^5)$ terms in (3). For a fixed steplength h, its general step, leading from x_{2n} to $x_{2n+2} = x_{2n} + 2h$, may be described as follows:

Given y_{2n}, z_{2n}, f_{2n} and f_{2n-1},

$$\text{(i)} \quad y_{2n+1} = y_{2n} + hz_{2n} + \frac{h^2}{6}(4f_{2n} - f_{2n-1}), \tag{4}$$

$$\text{(ii)} \quad f_{2n+1} = f(x_{2n+1}, y_{2n+1}), \tag{5}$$

$$\text{(iii)} \quad y_{2n+2} = y_{2n} + 2hz_{2n} + \frac{h^2}{3}(4f_{2n+1} + 2f_{2n}), \tag{6}$$

$$\text{(iv)} \quad f_{2n+2} = f(x_{2n+2}, y_{2n+2}), \tag{7}$$

$$\text{(v)} \quad z_{2n+2} = z_{2n} + \frac{h}{3}(f_{2n} + 4f_{2n+1} + f_{2n+2}). \tag{8}$$

The local truncation errors in y_{2n+2} and z_{2n+2} are of order h^5, and that in y_{2n+1} is of order h^4. This algorithm has some similarity with Runge-Kutta methods, but it involves only two function evaluations per step whereas a Runge-Kutta method of the same order requires three (see e.g. [10]). Unlike Runge-Kutta methods, the de Vogelaere algorithm is not self starting, but, as de Vogelaere [3] suggested, this difficulty is easily overcome since by taking

$$y_{-1} = y_0 - hz_0 + \frac{h^2}{2} f_0 \tag{9}$$

we can calculate f_{-1} with an error of order h^3.

An arbitrary change of steplength can be introduced without additional function evaluations. If a steplength h_1 is used as far as x_{2n}, the quantity f_{2n-1} refers to the mesh point $x_{2n-1} = x_{2n} - h_1$. If we now change the steplength to $h_2 = ch_1$, f_{2n-1} must be replaced in Eq. (4) by $\bar{f}_{2n-1}$, an approximation for f at $x_{2n} - h_2$. This can be achieved by defining

$$\bar{f}_{2n-1} = f_{2n} + c(f_{2n-1} - f_{2n}), \tag{10}$$

which has a local truncation error of order h_2^2.

3. Truncation Error Estimates. Equation (3) shows that the leading term in the truncation error in the step from x_{2n} to x_{2n+2} is

$$\frac{2h^5}{45} f'''_{2n}. \tag{11}$$

De Vogelaere [3] described a method for estimating this quantity when the steplength h is constant. To allow us to monitor the truncation error immediately after changes of steplength, it is necessary to introduce some modifications which are described in this section. We consider four separate cases.

3.1. *Fixed Steplength.* Since the truncation error in y_{2n+1} is of order h^4, and that in y_{2n+2} is of order h^5, $y(x_{2n+1})$ may be estimated more accurately by Taylor expansion about x_{2n}. By using the equations

$$h^2 f''_{2n+2} = f_{2n+2} - 2f_{2n+1} + f_{2n} + O(h^3)$$

and

$$hf'_{2n+2} = \frac{3}{2} f_{2n+2} - 2f_{2n+1} + \frac{1}{2} f_{2n} + O(h^3)$$

to replace the low-order derivatives, we obtain the new estimate

$$y^*_{2n+1} = y_{2n+2} - hz_{2n+2} + \frac{h^2}{24}(7f_{2n+2} + 6f_{2n+1} - f_{2n}), \tag{12}$$

which has a local truncation error of order h^5. Consequently,

$$y^*_{2n+1} - y_{2n+1} = \frac{h^4}{8} f''_{2n} + O(h^5). \tag{13}$$

Similarly, if the same steplength is used for the next step,

$$y^*_{2n+3} - y_{2n+3} = \frac{h^4}{8} f''_{2n+2} + O(h^5),$$

and the required truncation-error estimate is given by

$$\frac{2h^5}{45} f'''_{2n} \simeq \frac{h^4}{45} (f''_{2n+2} - f''_{2n})$$

$$\simeq \frac{8}{45} [(y^*_{2n+3} - y_{2n+3}) - (y^*_{2n+1} - y_{2n+1})].$$

The truncation error per unit step, which is a more appropriate basis for decisions about the steplength, is approximated by

$$\frac{4}{45h} [(y^*_{2n+3} - y_{2n+3}) - (y^*_{2n+1} - y_{2n+1})]. \tag{14}$$

3.2. *Immediately Following a Step Change.* Let h_1 be the steplength used in the step from x_{2n-2} to x_{2n}, and in the preceding step. Equations (6) and (8) can be used to put Eq. (12), with n replaced by $n - 1$, in the form

$$y^*_{2n-1} = y_{2n-2} + h_1 z_{2n-2} + \frac{1}{24} h_1^2 (7f_{2n-2} + 6f_{2n-1} - f_{2n}). \tag{15}$$

Then

$$\begin{aligned} y^*_{2n-1} - y_{2n-1} &= \frac{1}{24} h_1^2 (-9f_{2n-2} + 6f_{2n-1} - f_{2n} + 4f_{2n-3}) \\ &= \frac{h_1^4}{8} f''_{2n-1} - \frac{h_1^5}{6} f'''_{2n-1} + O(h_1^6). \end{aligned} \tag{16}$$

If the steplength is now changed to $h_2 = ch_1$ for the next step, Eq. (10) combines with (4) to give

$$y_{2n+1} = y_{2n} + h_2 z_{2n} + \frac{1}{6} h_2^2 [(3 + c) f_{2n} - c f_{2n-1}]. \tag{17}$$

Equations (6) and (8) apply with $h = h_2$, and

$$y^*_{2n+1} = y_{2n} + h_2 z_{2n} + \frac{1}{24} h_2^2 (7f_{2n} + 6f_{2n+1} - f_{2n+2}).$$

Steps similar to those used in deriving Eq. (16) then show that

$$y^*_{2n+1} - y_{2n+1} = \frac{h_2^4}{24}\left(1 + \frac{2}{c}\right) f''_{2n+1} - \frac{h_2^5}{36}\left(2 + \frac{3}{c} + \frac{1}{c^2}\right) f'''_{2n+1} + O(h_2^6), \tag{18}$$

and

$$(y^*_{2n+1} - y_{2n+1}) - \frac{1}{3} c^4 \left(1 + \frac{2}{c}\right) (y^*_{2n-1} - y_{2n-1})$$

$$= \frac{h_2^5}{72}\left(-1 + \frac{7}{c} + \frac{12}{c^2}\right) f'''_{2n} + O(h_2^6).$$

The resulting estimate of the truncation error per unit step is

$$\frac{8c[(y^*_{2n+1} - y_{2n+1}) - \alpha(y^*_{2n-1} - y_{2n-1})]}{5h_1(12 + 7c - c^2)}, \tag{19}$$

where

$$\alpha = \frac{1}{3}c^3(2 + c). \tag{20}$$

3.3. *The Second Step After a Step Change.* If the steplength $h_2 = ch_1$, introduced for the step from x_{2n} to x_{2n+2}, is retained in the next step, the equation

$$y^*_{2n+3} - y_{2n+3} = \frac{h_2^4}{8} f''_{2n+3} - \frac{h_2^5}{6} f'''_{2n+3} + O(h_2^6)$$

follows directly from (16). This combines with Eq. (18) to give

$$\begin{aligned} &\frac{1}{3}\left(1 + \frac{2}{c}\right)(y^*_{2n+3} - y_{2n+3}) - (y^*_{2n+1} - y_{2n+1}) \\ &\qquad = \frac{h_2^5}{36}\left(3 + \frac{5}{c} + \frac{1}{c^2}\right)f'''_{2n+2} + \cdots . \end{aligned} \tag{21}$$

The local truncation error per unit step is estimated to be

$$\frac{4c[\beta(y^*_{2n+3} - y_{2n+3}) - (y^*_{2n+1} - y_{2n+1})]}{5h_1(1 + 5c + 3c^2)} \tag{22}$$

with

$$\beta = \frac{1}{3}\left(1 + \frac{2}{c}\right).$$

If we now continue to use the steplength h_2 the results of Subsection 3.1 apply to later steps.

3.4. *Two Step Changes in Succession.* The alternative to the situation discussed in Subsection 3.3 is that having completed the step from x_{2n} to x_{2n+2} with steplength h_2 we then adopt a new steplength $h_3 = c_1h_2$. The relevant mesh points are

$$\begin{aligned} &x_{2n-1} = x_{2n} - h_1, \quad x_{2n}, \quad x_{2n+1} = x_{2n} + h_2, \\ &x_{2n+2} = x_{2n} + 2h_2, \quad x_{2n+3} = x_{2n+2} + h_3, \quad x_{2n+4} = x_{2n+2} + 2h_3. \end{aligned}$$

In this case, by analogy with Eq. (18),

$$y^*_{2n+3} - y_{2n+3} = \frac{h_3^4}{24}\left(1 + \frac{2}{c_1}\right)f''_{2n+3} - \frac{h_3^5}{36}\left(2 + \frac{3}{c_1} + \frac{1}{c_1^2}\right)f'''_{2n+3} + O(h_3^6). \tag{23}$$

The appropriate linear combination of (18) and (23) is

$$\beta(y^*_{2n+3} - y_{2n+3}) - \alpha_1(y^*_{2n+1} - y_{2n+1})$$

with

$$\beta = \frac{1}{3}\left(1 + \frac{2}{c}\right), \qquad \alpha_1 = \frac{1}{3}c_1^3(2 + c_1).$$

Our estimate for the local truncation error per unit step is then

$$\frac{24c^2c_1^2[\beta(y^*_{2n+3} - y_{2n+3}) - \alpha_1(y^*_{2n+1} - y_{2n+1})]}{5h_3[c^2(12 + 7c_1 - c_1^2) + c(20 + 12c_1 - 2c_1^2) + 2c_1 + 4]}. \tag{24}$$

4. A Bound for the Local Truncation Error. The error analysis described here is based on three functionals which are related to the truncation errors in the formulae (4), (6) and (8). For an arbitrary function $y(x)$, having $p + 1$ continuous derivatives, we define the functional

$$L_1[y(x), h] = y(x + h) - y(x) - hy'(x) - \frac{h^2}{6}[4y''(x) - y''(x - h)]. \tag{25}$$

By using Taylor's theorem in the form

$$y(x + jh) = y(x) + jhy'(x) + \cdots + \frac{(jh)^p}{p!}y^{(p)}(x) + \frac{h^{p+1}}{p!}\int_0^j (j - s)^p y^{(p+1)}(x)\,ds,$$

it can be shown that

$$L_1[y(x), h] = \frac{h^4}{6}\int_{-1}^1 G_1(s)y^{\text{iv}}(x + sh)\,ds \tag{26}$$

with

$$G_1(s) = \begin{cases} (1 + s), & -1 \leqslant s \leqslant 0, \\ (1 - s)^3, & 0 \leqslant s \leqslant 1. \end{cases}$$

Since $G_1(s)$ is of constant sign on the interval of integration, Eq. (26) may be written as

$$L_1[y(x), h] = h^4c_1y^{\text{iv}}(x + \theta_1 h), \qquad -1 < \theta_1 < 1, \tag{27}$$

with

$$c_1 = \frac{1}{6}\int_{-1}^1 G_1(s)\,ds = \frac{1}{8}.$$

The same approach applied to the functional

$$L_2[y(x), h] = y(x + 2h) - y(x) - 2hy'(x) - \frac{h^2}{3}[4y''(x + h) + 2y''(x)] \tag{28}$$

gives

$$L_2[y(x), h] = \frac{h^5}{4!}\int_0^2 G_2(s)y^{\text{v}}(x + sh)\,ds,$$

where

$$G_2(s) = \begin{cases} (2 - s)^4 - 16(1 - s)^2, & 0 \leqslant s \leqslant 1, \\ (2 - s)^4, & 1 \leqslant s \leqslant 2. \end{cases}$$

The kernel function $G_2(s)$ is of constant sign, and consequently

(29) $$L_2[y(x), h] = h^5 c_2 y^{\mathrm{v}}(x + \theta_2 h), \qquad 0 < \theta_2 < 2,$$

with

$$c_2 = \frac{1}{24}\int_0^2 G_2(s)\, ds = \frac{2}{45}.$$

The third functional required is

(30) $$L_3[y(x), h] = y'(x + 2h) - y'(x) - \frac{h}{3}[y''(x) + 4y''(x + h) + y''(x + 2h)],$$

and the standard expression for the truncation error in Simpson's rule gives

(31) $$L_3[y(x), h] = -\frac{h^5}{90} y^{\mathrm{vi}}(x + \theta_3 h), \qquad 0 < \theta_3 < 2.$$

Let $y(x)$ be the exact solution of our initial-value problem. To investigate the local truncation error in the step from x_{2n} to x_{2n+2} we suppose that the starting values at x_{2n} are exact, i.e.

$$y_{2n} = y(x_{2n}), \qquad z_{2n} = y'(x_{2n}),$$
$$f_{2n} = y''(x_{2n}), \qquad f_{2n-1} = y''(x_{2n-1}).$$

Then the truncation error at x_{2n+1} is

(32) $$\begin{aligned} y(x_{2n+1}) - y_{2n+1} &= L_1[y(x_{2n}), h] \\ &= \frac{h^4}{8} y^{\mathrm{iv}}(x_{2n} + \theta_1 h), \qquad -1 < \theta_1 < 1. \end{aligned}$$

Also, in view of the assumed starting values,

$$L_2[y(x_{2n}), h] = y(x_{2n+2}) - y_{2n} - 2hz_{2n} - \frac{h^2}{3}[4y''(x_{2n+1}) + 2f_{2n}],$$

and the truncation error at x_{2n+2} is

(33) $$y(x_{2n+2}) - y_{2n+2} = L_2[y(x_{2n}), h] + \frac{4h^2}{3}[y''(x_{2n+1}) - f_{2n+1}].$$

To obtain a bound on this error we assume a Lipschitz condition

(34) $$|f(x, y) - f(x, \eta)| \leqslant K|y - \eta|$$

for all x in the appropriate interval $[a, b]$ and all finite y and η. Then, if

$$|y^{\text{iv}}(x)| \leqslant M_4, \qquad |y^{\text{v}}(x)| \leqslant M_5, \qquad x \in [a, b],$$

Eq. (33) gives the bound

$$|y(x_{2n+2}) - y_{2n+2}| \leqslant \frac{2h^5}{45} M_5 + \frac{Kh^6}{6} M_4. \tag{35}$$

In a similar manner it can be shown that

$$\begin{aligned} y'(x_{2n+2}) - z_{2n+2} = {} & L_3[y(x_{2n}), h] + \frac{4h}{3}[y''(x_{2n+1}) - f_{2n+1}] \\ & + \frac{h}{3}[y''(x_{2n+2}) - f_{2n+2}], \end{aligned} \tag{36}$$

giving the bound

$$|y'(x_{2n+2}) - z_{2n+2}| \leqslant \frac{h^5}{90} M_6 + \frac{Kh^5}{18}(3 + Kh^2) M_4 + \frac{2Kh^6}{135} M_5, \tag{37}$$

where

$$|y^{\text{vi}}(x)| \leqslant M_6, \qquad x \in [a, b].$$

5. **Stability Analysis.** If $y(x)$ is the exact solution of the initial-value problem, the global truncation errors in the function and derivative values at the end of the nth de Vogelaere step are

$$\begin{aligned} y(x_{2n-1}) - y_{2n-1} &= e_n^{(1)}, \\ y(x_{2n}) - y_{2n} &= e_n^{(2)}, \\ y'(x_{2n}) - z_{2n} &= e_n^{(3)}/h. \end{aligned}$$

The factor of h in the third definition is introduced to simplify the form of later equations. Equation (4), combined with the definition of the functional L_1, gives

$$\begin{aligned} e_{n+1}^{(1)} = {} & e_n^{(2)} + e_n^{(3)} + \frac{2h^2}{3}[y''(x_{2n}) - f_{2n}] \\ & - \frac{h^2}{6}[y''(x_{2n-1}) - f_{2n-1}] + L_1[y(x_{2n}), h]. \end{aligned} \tag{38}$$

Similarly, from Eqs. (6) and (8) and the definitions of the corresponding functionals,

$$\begin{aligned} e_{n+1}^{(2)} = {} & e_n^{(2)} + 2e_n^{(3)} + \frac{4h^2}{3}[y''(x_{2n+1}) - f_{2n+1}] \\ & + \frac{2h^2}{3}[y''(x_{2n}) - f_{2n}] + L_2[y(x_{2n}), h] \end{aligned} \tag{39}$$

and

$$\begin{aligned} e_{n+1}^{(3)} = {} & e_n^{(3)} + \frac{h^2}{3}[y''(x_{2n}) - f_{2n} + 4\{y''(x_{2n+1}) - f_{2n+1}\} + y''(x_{2n+2}) - f_{2n+2}] \\ & + hL_3[y(x_{2n}), h]. \end{aligned} \tag{40}$$

In accordance with normal practice (e.g. Lambert [6, p. 257]) the stability of the method is discussed with reference to the equation

$$y'' = \lambda^2 y.$$

In this case our equations for the cumulative errors simplify to

$$A\mathbf{e}_{n+1} = B\mathbf{e}_n + \boldsymbol{\phi}_{n+1} \tag{41}$$

where $\mathbf{e}_n$ is a column vector with components $e_n^{(1)}$, $e_n^{(2)}$ and $e_n^{(3)}$, $\boldsymbol{\phi}_{n+1}$ has as its components the three functionals occurring in Eqs. (38)–(40), and the matrices A and B are

$$A = \begin{pmatrix} 1 & 0 & 0 \\ -\frac{4\bar{h}}{3} & 1 & 0 \\ -\frac{4\bar{h}}{3} & -\frac{\bar{h}}{3} & 1 \end{pmatrix}, \quad B = \begin{pmatrix} -\frac{\bar{h}}{6} & 1 + \frac{2\bar{h}}{3} & 1 \\ 0 & 1 + \frac{2\bar{h}}{3} & 2 \\ 0 & \frac{\bar{h}}{3} & 1 \end{pmatrix}$$

with $\bar{h} = \lambda^2 h^2$. Since A is nonsingular Eq. (41) may be written as

$$\mathbf{e}_{n+1} = C\mathbf{e}_n + A^{-1}\boldsymbol{\phi}_{n+1},$$

where

$$C = \begin{pmatrix} -\frac{\bar{h}}{6} & 1 + 2\frac{\bar{h}}{3} & 1 \\ -\frac{2\bar{h}^2}{9} & 1 + 2\bar{h} + \frac{8\bar{h}^2}{9} & 2\left(1 + \frac{2\bar{h}}{3}\right) \\ -\frac{2\bar{h}^2}{9}\left(1 + \frac{\bar{h}}{3}\right) & \frac{\bar{h}}{3}\left(6 + \frac{14\bar{h}}{3} + \frac{8\bar{h}^2}{9}\right) & 1 + 2\bar{h} + \frac{4\bar{h}^2}{9} \end{pmatrix}.$$

The characteristic polynomial of the matrix C is

$$p(r, \bar{h}) = 6r^3 - (12 + 23\bar{h} + 8\bar{h}^2)r^2 + (6 - 2\bar{h} - 4\bar{h}^2)r + \bar{h}.$$

The "Schur criterion" described on p. 78 of Lambert's book [6] can be used to show that $p(r, \bar{h})$ is a Schur polynomial, in other words that all its zeros lie inside the unit circle, if and only if $\bar{h} \in (-2, 0)$. Thus, the interval of absolute stability of de Vogelaere's method is $[-2, 0]$. The moduli of the zeros of $p(r, \bar{h})$ are plotted in Figure 1 for a range of values of $\bar{h}$. The three zeros, though distinct, have the same modulus when $\bar{h} = -1.732$ (to 3 decimal places).

6. The Cumulative Error. Bounds for the global truncation error can be obtained from Eqs. (38)–(40) and bounds established in Section 4. However, the dependence on a (fixed) steplength h is more readily obtained in an alternative approach described by Kopal [5, p. 219]. Let y be the exact solution of the initial-value problem

$$y'' = f(x, y), \quad y(x_0) = y_0, \quad z(x_0) = z_0$$

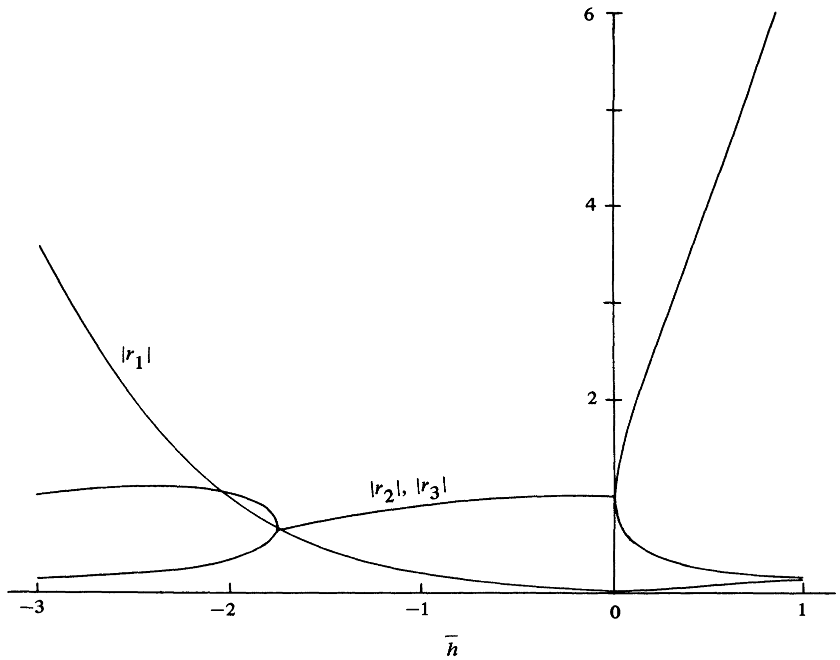

FIGURE 1
The moduli of the zeros r_1, r_2 and r_3 of $p(r, \bar{h})$. r_2 and r_3 are complex for $\bar{h} \in (-1.75, 0)$, and r_1 is always real

and z its derivative. Another solution of the differential equation is denoted by ξ and its derivative is η. Then, if the squares and higher powers of the differences $|\xi(x) - y(x)|$ and $|\eta(x) - z(x)|$ are neglected,

$$\frac{d}{dx}(\eta - z) = \frac{\partial f}{\partial y}(\xi - y), \qquad \frac{d}{dx}(\xi - y) = \eta - z. \tag{42}$$

When this is combined with the adjoint system

$$\lambda' = -\left(\frac{\partial f}{\partial y}\right)\mu, \qquad \mu' = -\lambda,$$

solved subject to the boundary conditions

$$\lambda(x_{2n}) = 1, \qquad \mu(x_{2n}) = 0,$$

Kopal's approach [5] gives the truncation-error estimate

$$y(x_{2n}) - y_{2n} \simeq \sum_{j=1}^{n} [\lambda(x_{2j})R_j + \mu(x_{2j})S_j]. \tag{43}$$

Here R_j and S_j represent the errors in evaluating the solution and its derivative in the jth step of the de Vogelaere method; more precisely

$$R_j = \xi_j(x_{2j}) - y_{2j}, \qquad S_j = \eta_j(x_{2j}) - z_{2j},$$

where $\xi_j(x)$ and $\eta_j(x)$ are the solutions of (42) on the interval $[x_{2j-2}, x_{2j}]$ satisfying the initial conditions

$$\xi_j(x_{2j-2}) = y_{2j-2}, \qquad \eta_j(x_{2j-2}) = z_{2j-2}.$$

Regarding the right-hand side of (43) as a quadrature sum we may write

$$y(x_{2n}) - y_{2n} \simeq \frac{1}{2h}\int_{x_0}^{x_{2n}} [\lambda(x)R(x) + \mu(x)S(x)]\, dx, \tag{44}$$

and only the lowest power of h in R and S is required for our purpose. From Eq. (3), or by retaining only the lowest power of h in (33), we obtain

$$R(x) = \frac{2h^5}{45} y^{\text{v}}(x).$$

The h^5 contribution to the local truncation error in the derivative comes from two sources, the first and second terms on the right-hand side of Eq. (36); thus,

$$S(x) = -\frac{h^5}{90} y^{\text{vi}}(x) + \frac{h^5}{6}\frac{\partial f}{\partial y} y^{\text{iv}}(x).$$

It follows from (44) that the global error is of order h^4.

As an example we consider the initial-value problem

$$y'' = -y, \qquad y(0) = 0, \qquad y'(0) = 1.$$

In this case

$$y(x) = \sin x, \qquad \lambda(x) = \cos(x_{2n} - x), \qquad \mu(x) = \sin(x_{2n} - x),$$

$$R(x) = \frac{2h^5}{45}\cos x, \qquad S(x) = -\frac{7h^5}{45}\sin x,$$

and the global error estimate is

$$\begin{aligned} y(x_{2n}) - y_{2n} &\simeq \frac{h^4}{90}\int_0^{x_{2n}} [2\cos(x_{2n} - x)\cos x - 7\sin(x_{2n} - x)\sin x]\, dx \\ &= \frac{h^4}{180}[9x_{2n}\cos x_{2n} - 5\sin x_{2n}]. \end{aligned}$$

In particular, when $x_{2n} = \pi/2$ this estimate becomes $-h^4/36$ which agrees closely with numerical results.

7. **Conclusion.** The truncation-error estimates presented in Section 3 provide a practical means of efficient error control in applications of de Vogelaere's method. The error estimates are inexpensive, requiring no extra function evaluations, and only two function evaluations are lost if a particular step has to be discarded. We have used this approach in a program for quantum mechanical scattering calculations, allowing the computer to choose the steplength at each step so that the truncation error per unit step is less, but not too much less, than a specified tolerance.

An important conclusion from our error analysis is that the global error in de Vogelaere's method is of order h^4. This contrasts with linear multistep methods for

Eq. (1) which have a local truncation error of order h^{p+2} but a global error of order h^p (see Henrici [4, p. 314]). For example, Numerov's method (Lambert [6, p. 255], Kopal [5, p. 183]) has a local truncation error of order h^6 but a global error of order h^4 like de Vogelaere's method.

Acknowledgement. This research was supported in part by a Research Grant from the Science Research Council.

Added in Proof. We have now established a rigorous upper bound on the global truncation error, assuming the Lipschitz condition and derivative bounds introduced in Section 4. For any $h_0 > 0$, constants a and M exist such that, for all $h \leqslant h_0$,

$$|y(x_{2n}) - y_{2n}| \leqslant \epsilon \exp[a(x_{2n} - x_0)] + \frac{\exp[a(x_{2n} - x_0)] - 1}{2a} h^4 M$$

where

$$\epsilon = \max\{|y(x_0) - y_0|, h|y(x_{-1}) - y_{-1}|, |z(x_0) - z_0|\}.$$

In particular, if the initial conditions of Section 2 are satisfied exactly, then

$$\epsilon = h|y(x_{-1}) - y_{-1}|,$$

which is of order h^4 if Eq. (9) is used to compute y_{-1}. Details will appear in Julie Mohamed's Ph.D. thesis.

Department of Mathematics
University of Durham
Durham, England

1. S. BASAVAIAH & R. F. BROOM, "Characteristics of in-line Josephson tunneling gates," *IEEE Trans. Magnetics*, v. MAG-11, 1975, pp. 759–762.

2. N. CHANDRA, "A general program to study the scattering of particles by solving coupled inhomogeneous second-order differential equations," *Computer Phys. Commun.*, v. 5, 1973, pp. 417–429.

3. R. de VOGELAERE, "A method for the numerical integration of differential equations of second order without explicit first derivatives," *J. Res. Nat. Bur. Standards*, v. 54, 1955, pp. 119–125.

4. P. HENRICI, *Discrete Variable Methods in Ordinary Differential Equations*, Wiley, New York, 1962.

5. Z. KOPAL, *Numerical Analysis*, Chapman and Hall, London, 1955.

6. J. D. LAMBERT, *Computational Methods in Ordinary Differential Equations*, Wiley, London, 1973.

7. J. D. LAMBERT, "The initial value problem for ordinary differential equations," in *The State of the Art in Numerical Analysis* (D. A. H. Jacobs, Editor), Academic Press, London, 1977, pp. 451–500.

8. J. -M. LAUNAY, "Body-fixed formulation of rotational excitation: exact and centrifugal decoupling results for CO – He," *J. Phys. B: Atom. Molec. Phys.*, v. 9, 1976, pp. 1823–1838.

9. W. A. LESTER, JR., "De Vogelaere's method for the numerical integration of second-order differential equations without explicit first derivatives: application to coupled equations arising from the Schrödinger equation," *J. Computational Phys.*, v. 3, 1968, pp. 322–326.

10. R. E. SCRATON, "The numerical solution of second-order differential equations not containing the first derivative explicitly," *Comput. J.*, v. 6, 1964, pp. 368–370.

11. L. F. SHAMPINE, H. A. WATTS & S. M. DAVENPORT, "Solving nonstiff ordinary differential equations—the state of the art," *SIAM Rev.*, v. 18, 1976, pp. 376–411.

12. L. VERLET, "Computer 'experiments' on classical fluids. I. Thermodynamical properties of Lennard-Jones molecules," *Phys. Rev.*, v. 159, 1967, pp. 98–103.