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# Linear Multistep Methods for Functional Differential Equations

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**Abstract.** A new way to define linear multistep methods for functional differential equations is presented, and some of their properties are analyzed. The asymptotic behavior of the global discretization error is investigated. Finally, Milne's device is generalized to functional differential equations. The effect of the nonsmoothness of the exact solution is taken into account.

**1. Introduction.** Consider the functional differential equation (FDE)

$$x'(t) = F(t, x_t) \qquad (t_0 \leqslant t \leqslant T),\ x_{t_0} = \phi, \tag{1}$$

where $x(t) \in \mathbf{R}^n$, $\phi \in C([-\tau, 0], \mathbf{R}^n)$, $F \in C([t_0, T] \times C([-\tau, 0], \mathbf{R}^n), \mathbf{R}^n)$ and $x_t$: $\theta \to x(t + \theta)$ for $\theta \in [-\tau, 0]$, $t \in [t_0, T]$. It is well known that the solution $x$ of (1) is usually not smooth, that is, even if $F$ and $\phi$ are $C^\infty$ functions, $x$ may have jump discontinuities in its derivatives. The occurrence of these jump discontinuities may lead to order-breakdown for numerical methods if no special provisions are made. It seems that all available techniques require information about the location of the jumps. If the delay is not state-dependent, then these locations may be known a priori. If not, then they may be calculated numerically (see Feldstein and Neves [6]).

When the location of a jump discontinuity is known, two different techniques are available:

(i) Make the location of the jump a grid point, and restart. In practice, this technique is only usable for delay-differential equations

$$x'(t) = F(t, x(t), x(t - \tau_1), \ldots, x(t - \tau_r))$$

and then it is quite efficient for one-step methods. (Note that the GBS-algorithm may integrate over a jump that lies on the grid without restart (see de Gee [8]).)

(ii) Calculate the height of the jump and subtract a piecewise polynomial $\chi$ from the solution $x$ such that the difference is a smooth function. This difference is then calculated by solving the FDE for that function. This technique is usable for one- and multistep methods, and also for more complicated FDEs than delay-differential equations.

This paper discusses linear multistep methods that use the jump correction technique as described in (ii) above.

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**2. The Construction of Linear Multistep Methods.** Throughout this paper the following assumptions are made:

A1. The FDE (1) has a solution $x$: $[t_0 - \tau, T] \to \mathbf{R}^n$ that is a piecewise smooth function, i.e., there are $s_1, \ldots, s_N \in [t_0 - \tau, T]$ such that $t \to x^{(m)}$ exists as a bounded continuous function on $[t_0 - \tau, T] \setminus \{s_1, \ldots, s_N\}$. Thus $x^{(j)}$ may have a jump discontinuity at $t = s_\nu$, $1 \leqslant \nu \leqslant N$, $1 \leqslant j \leqslant m$, and $x = x_{(m)} + \chi$, where $x_{(m)} \in C^m([t_0 - \tau, T], \mathbf{R}^n)$ and $\chi$ is a piecewise polynomial of degree $\leqslant m$. (Sufficient conditions on $F$ and $\phi$ for Assumption A1 may be found in de Gee [7].)

A2. $F$ is Lipschitzian with respect to its second variable: There are $\delta > 0$, $M_1 > 0$ such that for all $\psi_1, \psi_2 \in C([-\tau, 0], \mathbf{R}^n)$ with $\|\psi_1 - \psi_2\| \leqslant \delta$,

$$|F(t, \psi_1) - F(t, \psi_2)| \leqslant M_1 \|\psi_1 - \psi_2\|. \tag{2}$$

(This condition is sufficient for the uniqueness of the solution and for its continuous dependence with respect to perturbations in (1). Here and in many other places in this paper, constants $M$ may be replaced by Riemann-integrable functions $m$: $[t_0, T] \to \mathbf{R}^+$, at the cost of increased technical complexity of the proofs.)

Since the right-hand side $F(t, \cdot)$ of the FDE (1) may contain functionals on $C([-\tau, 0], \mathbf{R}^n)$ of continuous type, it is reasonable to allow $F$ to be approximated by another function $F_h$: $[t_0, T] \times C([-\tau, 0], \mathbf{R}^n) \to \mathbf{R}^n$. (This function may be thought of as being derived from $F$ by means of a discretization method. Thus, if $\psi = \chi + \psi_{(m)}$, with $\psi_{(m)} \in C^m([-\tau, 0], \mathbf{R}^n)$, and $\chi$ is a piecewise polynomial, one may replace $F(t, \psi) = \int_{-\tau}^{0} \psi(\theta)\, d\theta$ by $F_h(t, \psi) = \int_{-\tau}^{0} \chi(\theta) d\theta + Q_h(\psi_{(m)})$, where $Q_h$ is a quadrature method on $[-\tau, 0]$.) For $F_h$ we have the following assumptions:

A3. $F_h$ is uniformly Lipschitz continuous: There are $\delta > 0$, $h_0 > 0$, $M_2 > 0$ such that for all $\psi_1, \psi_2 \in C([-\tau, 0], \mathbf{R}^n)$ with $\|\psi_i - x_t\| < \delta$ and all $h \in (0, h_0]$,

$$|F_h(t, \psi_1) - F_h(t, \psi_2)| \leqslant M_2 \|\psi_1 - \psi_2\|. \tag{3}$$

A4. $F_h$ approximates $F$ on the graph $(t, x_t)$:

$$F_h(t, x_t) - F(t, x_t) = o(1) \quad \text{as } h \to 0, \text{ uniformly in } t \in [t_0, T]. \tag{4}$$

The mapping $F \to F_h$ will be called $\mathscr{D}$.

Besides the approximation of $F$ by $F_h$ (which in most cases amounts to approximation of continuous functionals by discrete functionals) we also need an approximation process to convert discrete functions to continuous functions. Let $u_j, v_j$: $[0,1] \to \mathbf{R}$ be continuous functions, $j = 0, \ldots, k$. Then an approximation scheme $\mathscr{A}$ is defined as follows: For any differentiable function $z$: $[a, b] \to \mathbf{R}^n$ the function

$$\mathscr{A}(r; z, t, h) = \sum_{j=0}^{k} \left[ u_j(r) z(t - jh) + h v_j(r) z'(t - jh) \right], \qquad r \in [0,1], \tag{5}$$

is (as function of $r$) an approximation of $z(t + (r-1)h)$ for any $t$ and $h$ such that $[t - kh, t] \subset [a, b]$. The approximation scheme is assumed to be consistent:

A5. For any differentiable function $z$: $[a, b] \to \mathbf{R}^n$ and any $t \in [a, b]$

$$\max |\mathscr{A}(r; z, t, h) - z(t + (r-1)h)| = o(1) \quad \text{as } h \to 0. \tag{6}$$

(Note that no uniformity in $z$ or $t$ is required.)

Finally, let $\mathscr{M}_0 = \{\alpha_j, \beta_j\}$ be a linear multistep method for ordinary differential equations:

$$\alpha_0 y_i + \cdots + \alpha_k y_{i-k} = h[\beta_0 f(t_i, y_i) + \cdots + \beta_k f(t_{i-k}, y_{i-k})]$$

yielding an approximation $y_i$ for the solution of the ODE $z'(t) = f(t, z(t))$ at $t = t_i$. The generating polynomials of $\mathscr{M}_0$ are $\rho$ and $\sigma$, respectively. $\mathscr{M}_0$ satisfies the usual assumptions of consistency and stability; in terms of $\rho$ and $\sigma$:

A6. $\rho(1) = 0$, $\sigma(1) = \rho'(1) \neq 0$.

A7. All roots $\lambda$ of $\rho$ satisfy $|\lambda| \leqslant 1$, and if $|\lambda| = 1$, then $\lambda$ is a simple root of $\rho$.

A multistep method $\mathscr{M}$ for (1) may now be defined as a quadruple $\mathscr{M} = \{\mathscr{M}_0, \mathscr{A}, \mathscr{D}, \chi\}$. $\mathscr{M}$ arises by substituting $\mathscr{A}$ into $\mathscr{M}_0$, and using the resulting recursion in $\mathbf{R}^n$ to approximate the values of the smooth part $x_{(m)} = x - \chi$:

$$\begin{aligned} &\sum_{j=0}^{k} \alpha_j [y(t_{i-j}) - \chi(t_{i-j})] = h \sum_{j=0}^{k} \beta_j [y'(t_{i-j}) - \chi'(t_{i-j})], \\ &y'(t_i) = F_h(t_i, P(t_i, y - \chi) + \chi_{t_i}), \\ &P(t, z)(\theta) = \sum_{j=0}^{k} [u_j(m + 1 + \theta/h) z(t - (j+m)h) \\ &\qquad\qquad + h v_j(m + 1 + \theta/h) z'(t - (j+m)h)], \\ &\qquad\qquad \theta \in [-(m+1)h, -mh],\ m = 0, \ldots, [\tau/h]. \end{aligned} \tag{7}$$

(Note that $P(t_l, y - \chi)$ approximates $(x - \chi)_{t_l}$, being the result of piecewise approximation by $\mathscr{A}$ on the iterates $y(t_{l-j})$, $j = 0, \ldots, [\tau/h] + k$, shifted back to $[-\tau, 0]$.)

The *local discretization error* of the multistep method $\mathscr{M}$ is given by

$$\begin{aligned} \delta_h(\mathscr{M}, t) = \sum_{j=0}^{k} \{ &\alpha_j [x - \chi](t - jh) \\ &- h\beta_j [F_h(t - jh, P(t - jh, x - \chi) + \chi_{t-jh}) - \chi'(t - jh)] \}. \end{aligned} \tag{8}$$

$\mathscr{M}$ is *consistent* for (1) if $\delta_h(\mathscr{M}, t) = o(h)$ uniformly as $h \to 0$, and it has consistency order $p$ if $\delta_h(\mathscr{M}, t) = O(h^{p+1})$ uniformly.

$\mathscr{M}$ is *stable* for (1) if for sufficiently small $h$, for any bounded family $\{\phi^{(h)}\} \subset C^1([-\tau, 0], \mathbf{R}^n)$ and any family $\{y(t_j), y'(t_j)\}_{0 \leqslant j \leqslant k-1}$ such that $\{y(t_j)\}$ and $\{y'(t_j)/h\}$ are uniformly bounded, the corresponding family $\{y(t_i)\}$ is bounded uniformly in $h$ and $i \leqslant (T - t_0)/h$.

$\mathscr{M}$ is *convergent* for (1) if for any family $\{\phi^{(h)}\} \subset C([-\tau, 0], \mathbf{R}^n)$ and any family $\{y(t_j), y'(t_j)\}_{0 \leqslant j \leqslant k-1}$ with

$$\|\phi^{(h)} - \phi\| = o(1), \tag{9a}$$

$$|y(t_j) - x(t_j)| = o(1), \tag{9b}$$

$$h|y'(t_j) - x'(t_j)| = o(1) \quad \text{as } h \to 0, \tag{9c}$$

the corresponding family $\{y(t_i)\}$ defined by (7) satisfies

$$|y(t_i) - x(t_i)| = o(1) \quad \text{as } h \to 0, \text{ uniformly in } i \leqslant (T - t_0)/h. \tag{9d}$$

It has *convergence order* $p$ if (9d) has $O(h^p)$ in the right-hand side whenever (9a)–(9c) have $O(h^p)$ in their right-hand sides.

THEOREM 1. a. *The multistep method* $\mathcal{M}$ *is consistent for* (1) *if*

(i) *the multistep method* $\mathcal{M}_0$ *for ODEs is consistent* (*Assumption* A6)

(ii) *the approximation scheme* $\mathcal{A}$ *is consistent*: $\sum u_j(r) = 1$ (*Assumption* A5)

(iii) $F_h(t, x_t) - F(t, x_t) = o(1)$ (*Assumption* A4)

(iv) $x - \chi$ *is differentiable and Lipschitzian*

(v) $F_h(t, \cdot)$ *is uniformly Lipschitzian* (*in the sense of Assumption* A3).

b. *The multistep method* $\mathcal{M}$ *is stable for* (1) *if*

(i) *the multistep method* $\mathcal{M}_0$ *is stable for ODEs* (*Assumption* A7)

(ii) $F_h(t, \cdot)$ *is uniformly Lipschitzian* (*in the sense of Assumption* A3).

c. *The multistep method* $\mathcal{M}$ *is convergent for* (1) *if it is stable and consistent, and it has convergence order p if it is stable and has consistency order p*.

d. *The multistep method* $\mathcal{M}$ *has consistency order p for* (1) *if*

(i) $\mathcal{M}_0$ *has consistency order p*

(ii) $\mathcal{A}$ *has consistency order* $p - 1$, *i.e., the right-hand side of* (6) *is* $O(h^p)$ *for any* $z \in C^{p-1}$ *with* $z^{(p-1)}$ *Lipschitzian*

(iii) $F_h(t, x_t) - F(t, x_t) = O(h^p)$ *uniformly*

(iv) $x - \chi \in C^{p-1}([t_0, T], \mathbf{R}^n)$, *and* $(x - \chi)^{(p-1)}$ *is Lipschitzian*

(v) $F_h(t, \cdot)$ *is uniformly Lipschitzian* (*in the sense of Assumption* A3). □

Theorem 1 shows that the properties of the various parts of which a linear multistep method is constructed are better preserved in $\mathcal{M}$ as defined in (7) than in the multistep methods considered by Tavernini [14]. Moreover, the construction (7) gives better opportunities to tune $\mathcal{A}$ and $\mathcal{D}$ to $F$.

**3. Asymptotic Behavior of the Global Discretization Error.** Consider the ordinary differential equation

$$z'(t) = f(t, z(t)), \qquad z(t_0) = z_0, \tag{10}$$

with exact solution $z(t)$. If $z_h(t)$ is the numerical solution obtained from a linear multistep method $\mathcal{M}_0$ with stepsize $h$, then (under conditions of smoothness of $z$ and the accuracy of the starting procedure) one usually has

$$z_h(t) - z(t) = h^p e_p(t) + O(h^{p+1}) \tag{11}$$

for some function $e_p$. In particular, if $z \in C^{p+1}$, then the local discretization error satisfies

$$\delta_h(\mathcal{M}_0, t) = C_{p+1} h^{p+1} z^{(p+1)}(t) + O(h^{p+2}), \tag{12}$$

and the function $e_p$ arises as a solution of the linearized problem along the solution curve of (10), with a forcing term proportional to $z^{(p+1)}$. If $z^{(p+1)}$ has a jump discontinuity, then (12) is no longer valid. Yet it will be shown that a result of the form (11) may still be obtained, for FDEs as well as for ODEs. For FDEs, where the solutions are rarely smooth, this means that we do not have to correct the jump discontinuities to a higher order for (11) than we have to for obtaining $p$th order convergence.

The following lemma describes the effect of a jump discontinuity in the $p$ + 1st derivative of the solution on the local discretization error of $\mathcal{M}_0$.

LEMMA 2. *Suppose that* $\mathcal{M}_0$ *is a k-step method for ODEs with order p and error constant* $C_{p+1}$, *i.e., the local discretization error of* $\mathcal{M}_0$ *for an ODE that has a* $C^\infty$ *solution z satisfies* (12). *Then the local discretization error of* $\mathcal{M}_0$ *for an ODE with a* *solution* $z \in C^p[t_0, T]$ *such that* $z^{(p)}$ *is Lipschitz continuous on* $[t_0, T]$ *and continuously differentiable on* $[t_0, T] \setminus \{s\}$, *satisfies*

$$(13)\quad \delta_h(\mathscr{M}_0, t) = C_{p+1}h^{p+1}z^{(p+1)}(t) + \gamma((t-s)/h)h^{p+1}\Delta z^{(p+1)} + O(h^{p+2}),$$

*where*

$$\Delta z^{(p+1)} = \lim_{\delta \downarrow 0}\left(z^{(p+1)}(s+\delta) - z^{(p+1)}(s-\delta)\right),$$

$$(14)\quad \gamma(r) = \sum_{j \geq r}^{k} \alpha_j (r-j)^{p+1}/(p+1)! - \beta_j (r-j)^p/p!.$$

*Proof.* Because $z^{(p+1)}$ is Riemann-integrable, the Taylor formulas

$$z(u) = \sum_{l=0}^{p} z^{(l)}(t)(u-t)^l/l! + \int_t^u (u-r)^p z^{(p+1)}(r)/p!\,dr,$$

$$z'(u) = \sum_{l=1}^{p} z^{(l)}(t)(u-t)^{l-1}/(l-1)! + \int_t^u (u-r)^{p-1} z^{(p+1)}(r)/(p-1)!\,dr$$

are valid. Because $\mathscr{M}_0$ has consistency order $p$, the polynomials do not contribute to $\delta_h(\mathscr{M}_0, t)$. Hence,

$$\delta_h(\mathscr{M}_0, t) = \sum_{j=0}^{k} \int_{t-jh}^{t} \big[-\alpha_j(t-jh-r)^p/p! + h\beta_j(t-jh-r)^{p-1}/(p-1)!\big] z^{(p+1)}(r)\,dr.$$

In the integrals we set $z^{(p+1)}(r) = z^{(p+1)}(t) + (1 - H_s(r))\Delta z^{(p+1)} + O(h)$, where $H_s$ is Heaviside's function at $s$. Thus for $s \leq t$,

$$\begin{aligned}\delta_h(\mathscr{M}_0, t) &= z^{(p+1)}(t) \sum_{j=0}^{k} \big[\alpha_j(-jh)^{p+1}/(p+1)! - h\beta_j(-jh)^p/p!\big] \\ &\quad + \Delta z^{(p+1)} \sum_{j \geq (t-s)/h}^{k} \int_{t-jh}^{t} \big[\alpha_j(t-jh-r)^p/p! - h\beta_j(t-jh-r)^{p-1}/(p-1)!\big]\,dr \\ &\quad + O(h^{p+2}) \\ &= C_{p+1}h^{p+1}z^{(p+1)}(t) + \gamma((t-s)/h)h^{p+1}\Delta z^{(p+1)} + O(h^{p+2}). \quad \square\end{aligned}$$

*Remarks on Lemma* 2.

1. The function $\gamma$ is a primitive of the function $G$ in Lambert [11, p. 50 ff.].

2. Formula (13) is not an expansion in $h$ of the local discretization error in the usual sense, because the argument of $\gamma$ depends on $h$.

3. Although not valid in general, for many widely used methods the relation $\max|\gamma(r)| = |C_{p+1}|$ turns out to be true. In Figures 1–4, $\gamma$ has been plotted for
   - the Adams-Bashforth schemes of order $p = 1, \ldots, 9$ (thus $k = p$);
   - the Adams-Moulton schemes of order $p = 1, \ldots, 9$ (thus $k = 1$ for $p = 1$, $k = p - 1$ for $p > 1$);
   - the implicit backward-difference schemes of order $p = 1, \ldots, 6$ (thus $k = p$);
   - the explicit midpoint rule and Simpson's rule.

These figures show how nicely $|\gamma(r)|$ tapers off from $|C_{p+1}|$ at $r = 0$ to 0 at $r = k$.

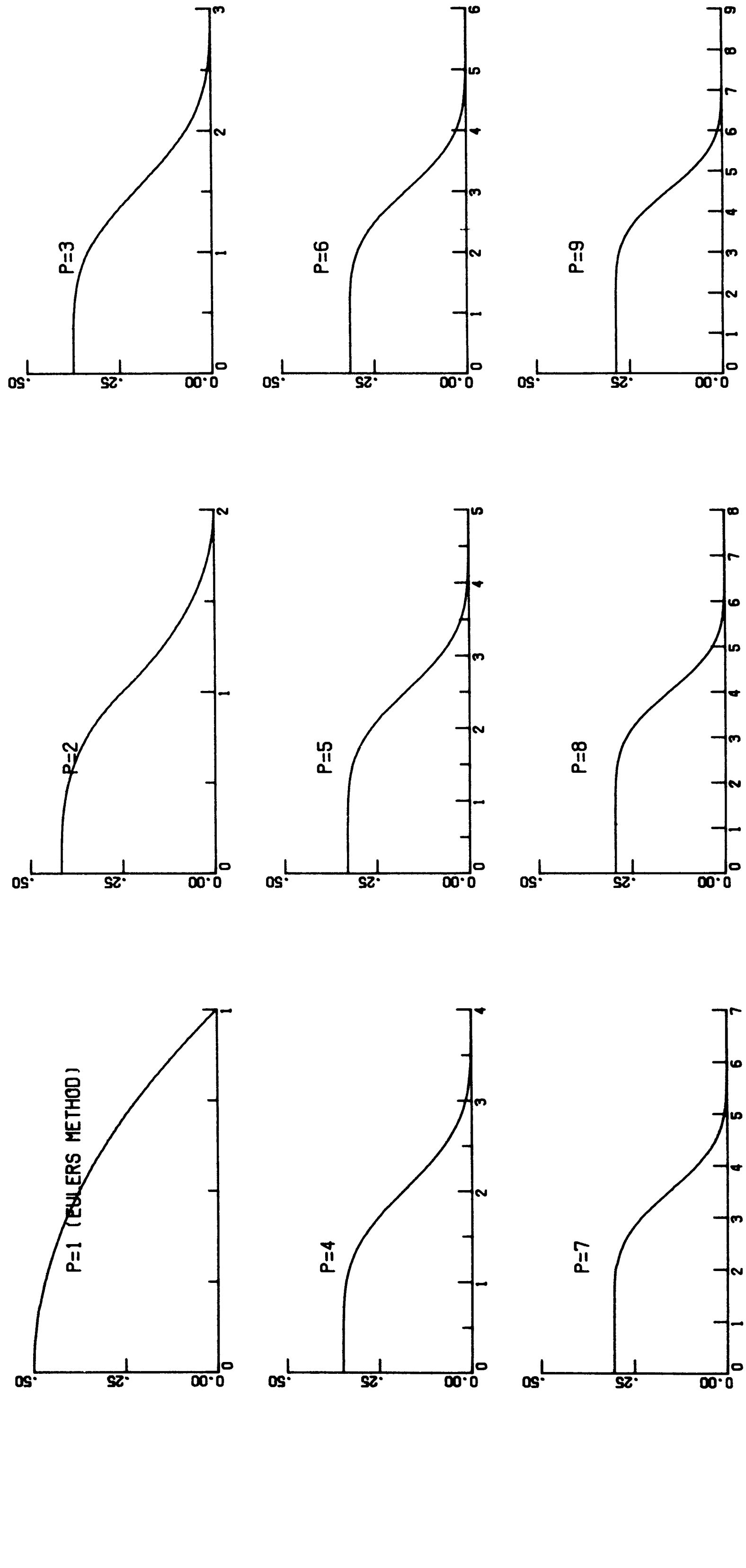


FIGURE 1

*The function γ for the Adams-Bashforth methods.*

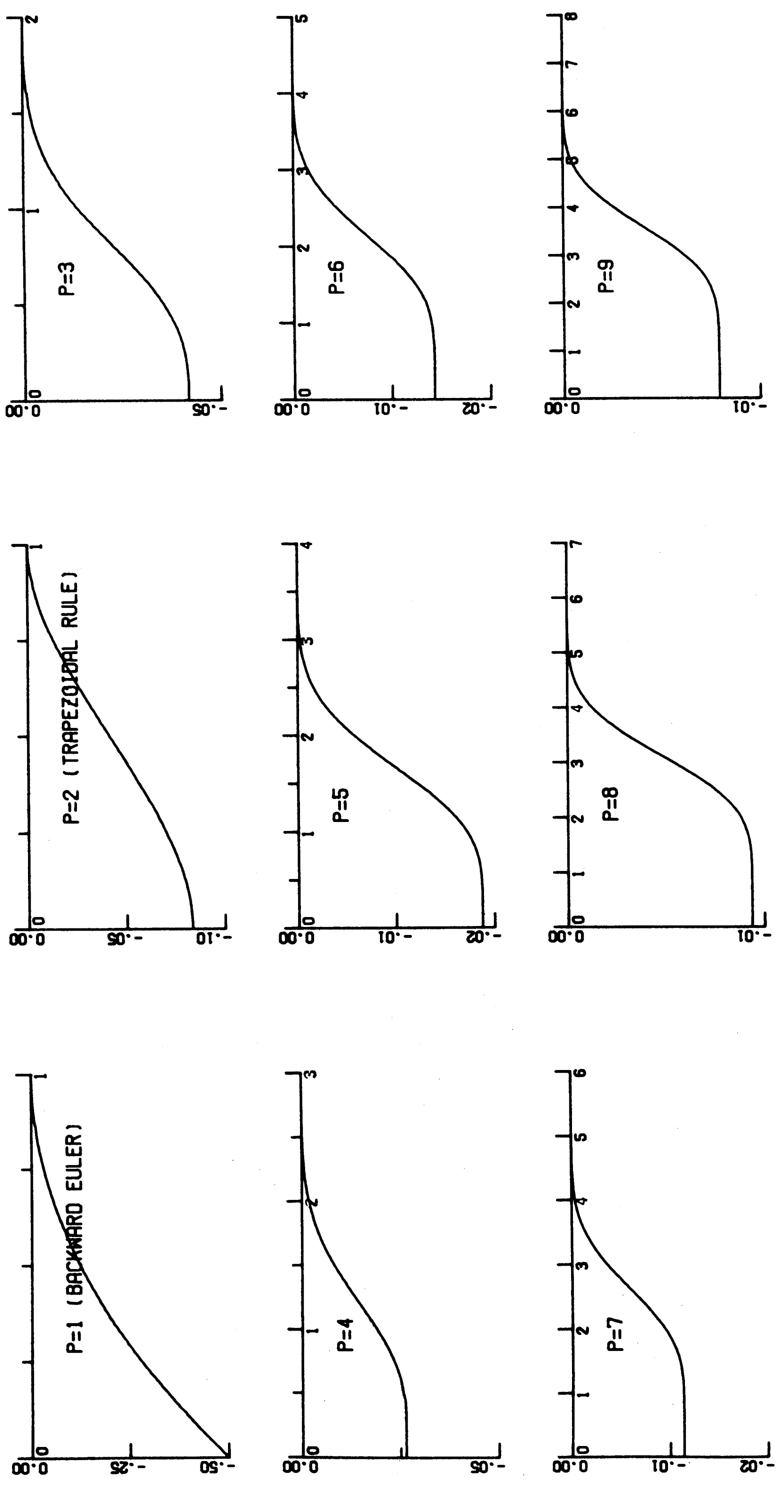


FIGURE 2
*The function γ for the Adams-Moulton methods.*

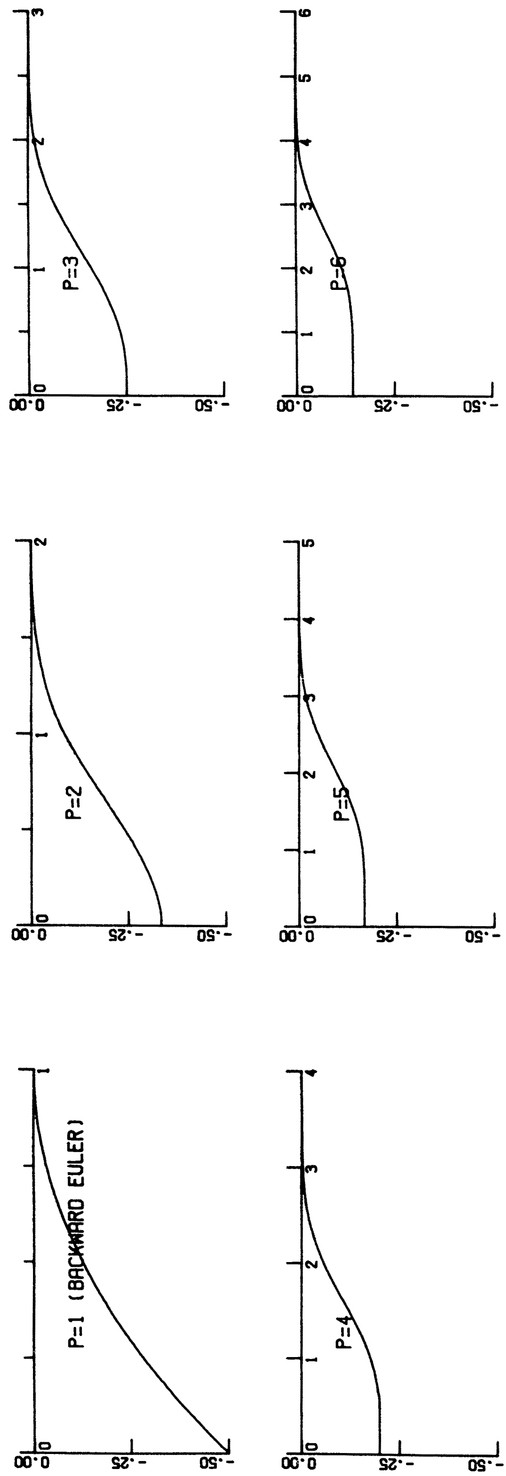


FIGURE 3

*The function γ for the backward-difference methods.*

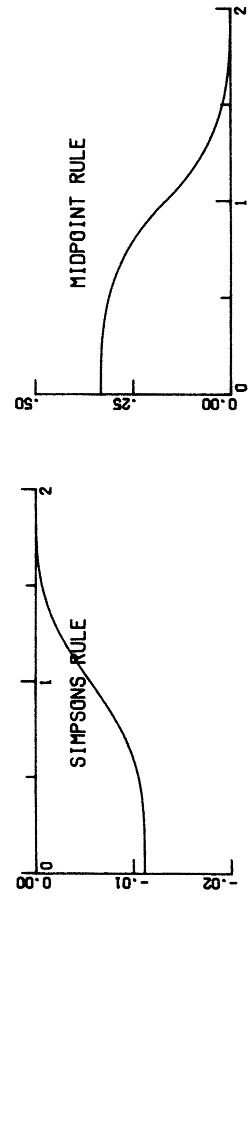


FIGURE 4

*The function γ for Simpson's rule and midpoint rule.*

We now present a theorem on the asymptotic behavior (for $h \to 0$) of the global discretization error of the multistep method $\mathscr{M}$. This requires somewhat stronger conditions on the FDE than those we have made in Section 2. So we replace the Assumptions A1–A4 by the following:

A1′. The FDE (1) has a solution $x$ such that $x = x_{(p)} + \chi$, where $\chi$ is a piecewise polynomial of degree $\leqslant p$, and $x_{(p)} \in C^p([t_0, T], \mathbf{R})$. $x_{(p)}^{(p)}$ is piecewise continuously differentiable with bounded derivative, which may have a finite number of jumps.

A2′. $F(t, \cdot)$ is Fréchet-differentiable on the graph $(t, x_t)$. The partial derivative, denoted by $L(t) = \partial F(t, \psi)_{\psi = x_t}/\partial\psi$ is bounded:

$$\|L(t)\| \leqslant M_1. \tag{15}$$

A3′. $F_h(t, \cdot)$ is continuously differentiable: There are $\varepsilon > 0$, $h_0 > 0$ and $M_2 > 0$ such that for all $\psi_i \in C([-\tau, 0], \mathbf{R}^n)$ with $\|\psi_i - x_t\| \leqslant \varepsilon$ and all $h \in (0, h_0]$,

$$\left\| \frac{\partial}{\partial\psi} F_h(t, \psi_1) - \frac{\partial}{\partial\psi} F_h(t, \psi_2) \right\| \leqslant M_2 \|\psi_1 - \psi_2\|. \tag{16}$$

A4′. There is a bounded, piecewise continuous function $l$: $[t_0, T] \to \mathbf{R}^n$ such that

$$F_h(t, x_t) - F(t, x_t) = h^p l(t) + O(h^{p+1}), \quad \text{uniformly in } t \in [t_0, T]. \tag{17}$$

Furthermore, for any compact subset $\mathscr{U} \subset C([t_0 - \tau, T], \mathbf{R}^n)$,

$$\frac{\partial}{\partial\psi} F_h(t; x_t) u_t - L(t) u_t = O(h), \quad \text{uniformly in } u \in \mathscr{U} \text{ and } t \in [t_0, T]. \tag{18}$$

(Again, the constants $M_1$, $M_2$ and the hidden constants in (17) and (18) may be replaced by Riemann-integrable functions; $l$ may be Riemann-integrable too.)

THEOREM 3. *Let $p \geqslant 1$. Let the families*

$$\{\phi^{(h)}\} \subset C([-\tau, 0], \mathbf{R}^n), \qquad \{y(t_j), y'(t_j)\}_{0 \leqslant j \leqslant k-1}$$

*be such that*

$$\|\phi^{(h)} - \phi\| = O(h^{p+1}), \quad |y(t_j) - x(t_j)| = O(h^{p+1}), \quad |y'(t_j) - x'(t_j)| = O(h^p).$$

*Let $\mathscr{M}_0$ be a stable linear k-step method for ODEs of consistency order p, with generating polynomials $\rho$ and $\sigma$ and error constant $c = C_{p+1}/\sigma(1)$. Let $\mathscr{A}$ be an approximation scheme of order p. Let $\mathscr{D}$ be the mapping $F \to F_h$, satisfying* A2′–A4′. *Let x be the solution of* (1), *satisfying* A1′. *Let $\{y(t_i)\}$ be the numerical solution of* (1), *generated by $\mathscr{M} = \{\mathscr{M}_0, \mathscr{A}, \mathscr{D}, \chi\}$ with stepsize h. Let $e_p$: $[t_0 - \tau, T] \to \mathbf{R}^n$ be the solution of the linear FDE*

$$e_p'(t) = L(t)(e_p)_t + l(t) - c x^{(p+1)}(t), \qquad (e_p)_{t_0} = 0. \tag{19}$$

*Then the global discretization error* $e(t_i) = y(t_i) - x(t_i)$ *satisfies*

$$e(t_i) = h^p e_p(t_i) + O(h^{p+1}). \tag{20}$$

*Proof.* On account of Theorem 1, $y(t_i) - x(t_i) = O(h^p)$ uniformly, and because $\mathscr{A}$ has order $p$, $\|x_{t_i} - \chi_{t_i} - P(t_i, x - \chi)\| = O(h^{p+1})$. Hence,

$$\begin{aligned}
F_h&\big(t_i, P(t_i, y-\chi) + \chi_{t_i}\big) - F(t_i, x_{t_i})\\
&= F_h\big(t_i, P(t_i, y-\chi) + \chi_{t_i}\big) - F_h\big(t_i, P(t_i, x-\chi) + \chi_{t_i}\big)\\
&\quad + F_h\big(t_i, P(t_i, x-\chi) + \chi_{t_i}\big) - F_h(t_i, x_{t_i}) + F_h(t_i, x_{t_i}) - F(t_i, x_{t_i})\\
&= \frac{\partial}{\partial\psi} F_h\big(t_i, P(t_i, x-\chi) + \chi_{t_i}\big) P(t_i, x_{t_i}) + O\Big(\|P(t_i, x-y)\|^2\Big)\\
&\quad + \frac{\partial}{\partial\psi} F(t_i, x_{t_i})\big(x_{t_i} - \chi_{t_i} - P(t_i, x-\chi)\big)\\
&\quad + O\Big(\|x_{t_i} - \chi_{t_i} - P(t_i, x-\chi)\|^2\Big) + h^p l(t_i) + O(h^{p+1})\\
&= \frac{\partial}{\partial\psi} F_h\big(t_i, P(t_i, x-\chi) - \chi_{t_i}\big) P(t_i, x-y) + h^p l(t_i) + O(h^{p+1})\\
&= \frac{\partial}{\partial\psi} F_h(t_i, x_{t_i}) P(t_i, x-y) + h^p l(t_i) + O(h^{p+1})\\
&= L(t_i) P(t_i, x-y) + h^p l(t_i) + O(h^{p+1}).
\end{aligned}$$

The last step is justified because all functions of the form $P(t_i, x-y)$ are linear combinations, with coefficients that are $O(h^p)$ in magnitude, of the functions $u_j$, $v_j$ of $\mathscr{A}$. Hence the family $\{h^{-p}P(t_i, x-y)\}$ is bounded and equicontinuous, and therefore relatively compact. Thus (18) may be used.

The global discretization error satisfies

$$\begin{aligned}
\sum_{j=0}^{k} \alpha_j e(t_{i-j}) &= \sum_{j=0}^{k} \alpha_j [y-\chi](t_{i-j}) - \sum_{j=0}^{k} \alpha_j [x-\chi](t_{i-j})\\
&= h \sum_{j=0}^{k} \beta_j \Big[F_h\big(t_{i-j}, P(t_{i-j}, y-\chi) + \chi_{t_{i-j}}\big) - F\big(t_{i-j}, x_{t_{i-j}}\big)\Big]\\
&\quad + h \sum_{j=0}^{k} \beta_j [x-\chi]'(t_{i-j}) - \sum_{j=0}^{k} \alpha_j [x-\chi](t_{i-j})\\
&= h \sum_{j=0}^{k} \beta_j \big[L(t_{i-j}) P(t_{i-j}, e) + h^p l(t_{i-j})\big]\\
&\quad + h^{p+1}\Big[C_{p+1} x^{(p+1)}(t_i) + \sum \gamma((t - s_\nu)/h) \Delta_\nu x^{(p+1)}\Big] + O(h^{p+2}),
\end{aligned}$$

where $\{s_\nu\}$ are the jumps of $x^{(p+1)}$. Writing $\tilde{e}(t_i) = e(t_i)/h^p$ we find that for all $i$ such that $x^{(p+1)}$ has no jumps in $[t_i, t_{i+k}]$,

$$\sum_{j=0}^{k} \alpha_j \tilde{e}(t_{i-j}) = h \sum_{j=0}^{k} \beta_j \big[L(t_{i-j}) P(t_{i-j}, \tilde{e}) + l(t_{i-j}) - c x^{(p+1)}(t_{i-j})\big] + O(h^2), \tag{21}$$

while for those $i$ for which $x^{(p+1)}$ has one or more jumps in $[t_i, t_{i+k}]$,

$$\sum_{j=0}^{k} \alpha_j \tilde{e}(t_{i-j}) = O(h).$$

Since $x^{(p+1)}$ has a finite number of jumps, (21) holds for all but a finite number of $i$, uniformly in $h \in (0, h_0]$. On the other hand, (21) is—up to a perturbation $O(h^2)$—the result of the multistep method $\{\mathscr{M}_0, \mathscr{A}, -, -\}$ applied to the FDE (19). A slightly modified form of Theorem 1 (to deal with the perturbations; compare, e.g., Tavernini [14, Lemma 3]) is now used to show that $\tilde{e}(t_i) = e_p(t_i) + O(h)$, which completes the proof. □

*Remarks on Theorem* 3.

1. It will be clear that A1′–A4′ imply A1–A4.

2. Comparison of the conditions of Theorem 3 with those of Theorem 1 shows that:
   - the smoothness conditions on $F$ and $F_h$ are made somewhat stronger, as well as the conditions of convergence of $F_h$ to $F$, but
   - the order of convergence of $F_h$ to $f$ remains the same;
   - the order of the multistep method $\mathscr{M}_0$ remains the same;
   - the smoothness conditions on $x$ between the jumps of its derivatives are made stronger, but
   - the number of derivatives for which the jumps are taken into account remains the same;
   - the order of the approximation scheme $\mathscr{A}$ is one higher in Theorem 3 than in Theorem 1. So by a different argument we come to the same conclusion as Arndt [1], [2]: For asymptotic error estimates and stepsize control of a $p$th order method, one should use an approximation scheme that has an order higher by 1 than is necessary to obtain $p$th order itself.

**4. Predictor-Corrector Methods and Milne's Device.** Results of the form (11) are often used locally in ODE solvers for stepsize control. Basically, there are two ways to use (11) to this end:

a. By comparing two approximations of different order. Examples are:
   - Runge-Kutta-Fehlberg algorithms (cf. Fehlberg [5]). For generalizations to delay-differential equations, see Oberle and Pesch [12] and Oppelstrup [13].
   - The Gragg-Bulirsch-Stoer algorithm (cf. Bulirsch and Stoer [4]). For a generalization to delay-differential equations, see de Gee [8], [9].

b. By comparing two approximations of the same order, for example in a predictor-corrector scheme. In this case the technique that yields an estimate for the local error is called Milne's device. In practice, a predictor-corrector is mostly used in $P_{k+1}EC_kE$ mode, where $P_{k+1}$ and $C_k$ are a $k+1$st order Adams-Bashforth-Moulton pair. In [3], Bock and Schlöder have reported on a code (REBUS) for delay-differential equations using predictor-corrector methods with Milne's device. However, no details are given.

In this section Milne's device is generalized to multistep methods $\mathscr{M}$ for FDEs. To avoid technical complications, the underlying multistep methods for ODEs are assumed to be Adams-Bashforth-Moulton pairs of the same order. Some justification lies in the fact that these are by far the most widely used methods.

Let for $k \geqslant 2$, $\tilde{\mathscr{M}}_0$ be the $k$th order Adams-Bashforth formula and $\mathscr{M}_0$ be the $k$th order Adams-Moulton formula for ODEs. Their generating polynomials are $(\tilde{\rho}, \tilde{\sigma})$ and $(\rho, \sigma)$, respectively:

$$\tilde{\rho}(\lambda) = \lambda^k(\lambda - 1), \quad \tilde{\sigma}(\lambda) = \sum_{j=1}^{k+1} \tilde{\beta}_j \lambda^{k-j+1},$$

$$\rho(\lambda) = \lambda^{k-1}(\lambda - 1), \quad \sigma(\lambda) = \sum_{j=0}^{k} \beta_j \lambda^{k-j}.$$

Let $\mathscr{A}$ be an approximation scheme of the form (5) that does not use $z'(t)$ as a known value, i.e., $v_0(r) = 0$, $r \in [0,1]$. Then the following relations define a $P_{k+1}EC_kE$ method for FDEs:

$$\tag{22} \begin{aligned} \tilde{y}(t_i) &= y(t_{i-1}) - \chi(t_{i-1}) + \chi(t_i) + h \sum_{j=1}^{k+1} \tilde{\beta}_j \left[ y'(t_{i-j}) - \chi'(t_{i-j}) \right], \\ \tilde{P}(t_i, z, \tilde{z}_i) &= \begin{cases} u_0(1 + \theta/h)\tilde{z}_i + \sum_{j=1}^{k} \left[ u_j(1 + \theta/h) z_{i-j} + h v_j(1 + \theta/h) z'_{i-j} \right], \\ \qquad\qquad \theta \in [-h, 0], \\ P(t_i, z), \qquad \theta \in [-\tau, -h), \end{cases} \\ \tilde{y}'(t_i) &= F_h\left(t_i, \tilde{P}(t_i, y - \chi, \tilde{y}(t_i) - \chi(t_i)) + \chi_{t_i}\right), \\ y(t_i) &= y(t_{i-1}) - \chi(t_{i-1}) + \chi(t_i) \\ &\quad + h \left[ \beta_0 \left( \tilde{y}'(t_i) - \chi'(t_i) \right) + \sum_{j=1}^{k} \beta_j \left( y'(t_{i-j}) - \chi'(t_{i-j}) \right) \right], \\ y'(t_i) &= F_h\left(t_i, P(t_i, y - \chi) + \chi_{t_i}\right). \end{aligned}$$

As before, $x$ is the solution of (1). Define $\tilde{x}$ by

$$\begin{aligned} \tilde{x}(t) &= x(t - h) - \chi(t - h) + \chi(t) \\ &\quad + h \sum_{j=1}^{k+1} \tilde{\beta}_j \left[ F_h\left(t - jh, P(t - jh, x - \chi) + \chi_{t-jh}\right) - \chi'(t - jh) \right]. \end{aligned}$$

Then $\delta_h(\mathscr{M}_p, t) = x(t) - \tilde{x}(t)$ is the local discretization error of the predictor for FDEs, cf. (8). Similarly,

$$\begin{aligned} \delta_h(\mathscr{M}_c, t) &= x(t) - \chi(t) - x(t - h) + \chi(t - h) \\ &\quad - h \sum_{j=0}^{k} \beta_j \left[ F_h\left(t - jh, P(t - jh, x - \chi) + \chi_{t-jh}\right) - \chi'(t - jh) \right] \end{aligned}$$

is the local discretization error of the corrector method for FDEs, and

$$\delta_h(\mathcal{M}_{pc}, t) = x(t) - \chi(t) - x(t-h) + \chi(t-h)$$
$$- h\beta_0\big[F_h(t, \tilde{P}(t, x-\chi, \tilde{x}(t) - \chi(t)) + \chi_t) - \chi'(t)\big]$$
$$- h\sum_{j=1}^{k}\beta_j\big[F_h\big(t - jh, P(t-jh, x-\chi) + \chi_{t-jh}\big) - \chi'(t-jh)\big]$$

is the local discretization error of the predictor-corrector method (22). From these definitions it is easily shown that under the conditions of Theorem 3,

$$\delta_h(\mathcal{M}_{pc}, t) = \delta_h(\mathcal{M}_c, t) + O(h^{k+2}). \tag{23}$$

Furthermore, a straightforward variation of the proof of Theorem 3 shows that the predictor-corrector method (22) has a global discretization error

$$e(t_i) = y(t_i) - x(t_i) = O(h^k), \quad \text{uniformly in } i \leqslant (T - t_0)/h. \tag{24}$$

LEMMA 4. *Let the assumptions of Theorem* 3 *be satisfied. Assume, moreover, that the function* $t \mapsto L(t)$ *in* A2′ *is Lipschitzian. Then*

$$y(t_i) - \tilde{y}(t_i) = \delta_h(\mathcal{M}_c, t_i) - \delta_h(\mathcal{M}_p, t_i)$$
$$+ O(h^{k+2}), \quad \textit{uniformly in } i \leqslant (T - t_0)/h.$$

*Proof*. If we set $\beta_{k+1} = \tilde{\beta}_0 = 0$, then the coefficients $\beta_j$ and $\tilde{\beta}_j$ of $\sigma$ and $\tilde{\sigma}$ satisfy the relations $\beta_j - \tilde{\beta}_j = (-1)^j\binom{k+1}{j}\beta_0$, $j = 0, \ldots, k+1$. Furthermore,

$$
\begin{aligned}
y(t_i) - \tilde{y}(t_i) &= h\beta_0\tilde{y}'(t_i) + h\sum_{j=1}^{k+1}(\beta_j - \tilde{\beta}_j)y'(t_{i-j}) \\
&= h\sum_{j=0}^{k+1}(\beta_j - \tilde{\beta}_j)y'(t_{i-j}) - h\beta_0(y'(t_i) - \tilde{y}'(t_i)) \\
&= h\sum_{j=0}^{k+1}(\beta_j - \tilde{\beta}_j)\Big[F_h\big(t_{i-j}, P(t_{i-j}, y-\chi) + \chi_{t_{i-j}}\big) \\
&\qquad - F_h\big(t_{i-j}, P(t_{i-j}, x-\chi) + \chi_{t_{i-j}}\big)\Big] \\
&\quad + h\sum_{j=0}^{k+1}(\beta_j - \tilde{\beta}_j)F_h\big(t_{i-j}, P(t_{i-j}, x-\chi) + \chi_{t_{i-j}}\big) \\
&\quad - h\beta_0(y'(t_i) - \tilde{y}'(t_i)) \\
&= h\sum_{j=0}^{k+1}(\beta_j - \tilde{\beta}_j)\Big[F_h\big(t_{i-j}, P(t_{i-j}, y-\chi) + \chi_{t_{i-j}}\big) \\
&\qquad - F_h\big(t_{i-j}, P(t_{i-j}, x-\chi) + \chi_{t_{i-j}}\big)\Big] \\
&\quad + \delta_h(\mathcal{M}_c, t_i) - \delta_h(\mathcal{M}_p, t_i) - h\beta_0(y'(t_i) - \tilde{y}'(t_i)).
\end{aligned}
\tag{25}
$$

Now consider the last sum on the right. It may be rewritten as

$$h\sum_{j=0}^{k+1}(\beta_j-\tilde{\beta}_j)\Big[F_h\big(t_{i-j},P(t_{i-j},y-\chi)+\chi_{t_{i-j}}\big)$$
$$-F_h\big(t_{i-j},P(t_{i-j},x-\chi)+\chi_{t_{i-j}}\big)\Big]$$
$$=h\sum_{j=0}^{k+1}(\beta_j-\tilde{\beta}_j)\Big[L(t_{i-j})P(t_{i-j},y-x)+O\big(\max|y(t_l)-x(t_l)|^2\big)$$
$$+O\big(h\max|y(t_l)-x(t_l)|\,\|x_{t_{i-j}}-\chi_{t_{i-j}}-P(t_{i-j},x-\chi)\|\big)\Big]$$
$$=h\sum_{j=0}^{k+1}(\beta_j-\tilde{\beta}_j)L(t_{i-j})P(t_{i-j},e)+O(h^{2k+1}) \tag{26}$$
$$=h\beta_0\sum_{j=0}^{k+1}(-1)^j\binom{k+1}{j}L(t_{i-j})P(t_{i-j},e)+O(h^{2k+1})$$
$$=h\beta_0\sum_{j=0}^{k}(-1)^j\binom{k}{j}\Big[L(t_{i-j})\big(P(t_{i-j},e)-P(t_{i-j-1},e)\big)$$
$$+\big(L(t_{i-j})-L(t_{i-j-1})\big)P(t_{i-j-1},e)\Big]+O(h^{2k+1})$$
$$=O\big(h\max|e_l-e_{l-1}|\big)+O\big(h^2\max|e_l|\big)+O(h^{2k+1}).$$

By definition of $e$,

$$e(t_i)-e(t_{i-1})=h\sum_{j=0}^{k}\beta_j\Big[F_h\big(t_{i-j},\tilde{P}(t_{i-j},x-\chi,(\tilde{x}-\chi)(t_{i-j}))+\chi_{t_{i-j}}\big)$$
$$-F_h\big(t_{i-j},\tilde{P}(t_{i-j},y-\chi,(\tilde{y}-\chi)(t_{i-j}))+\chi_{t_{i-j}}\big)\Big]$$
$$+\delta_h(\mathcal{M}_{pc},t_i)$$
$$=h\sum_{j=0}^{k}\beta_jO\big(\max|e_l|+|\delta_h(\mathcal{M}_p,t_i)|\big)+\delta_h(\mathcal{M}_{pc},t_i)=O(h^{k+1}),$$

because $|e_i|=O(h^k)$ and $\delta_h(\mathcal{M}_p,t)=O(h^{k+1})$, $\delta_h(\mathcal{M}_{pc},t)=O(h^{k+1})$. Thus we find that (26) is $O(h^{k+2})$. Substitution of this result in (25) yields

$$y(t_i)-\tilde{y}(t_i)=\delta_h(\mathcal{M}_c,t_i)-\delta_h(\mathcal{M}_p,t_i)-h\beta_0\big(y'(t_i)-\tilde{y}'(t_i)\big)+O(h^{k+2}),$$

from which the assertion follows. □

THEOREM 5 (Milne's device). *Let the assumptions of Lemma 4 be satisfied. Let the functions $\gamma$ and $\tilde{\gamma}$ be defined as in Lemma 2, corresponding to the corrector and the predictor, respectively; $C_{k+1}$ and $\tilde{C}_{k+1}$ are the leading constants in the expansion of the local discretization errors. Then*

$$\frac{C_{k+1}}{C_{k+1}-\tilde{C}_{k+1}}(y_i-\tilde{y}_i)$$
$$=\delta_h(\mathcal{M}_{pc},t_i)$$
$$+\sum_{\nu}\big[\tilde{C}_{k+1}\gamma((t_i-s_\nu)/h)-C_{k+1}\tilde{\gamma}((t_i-s_\nu)/h)\big]\Delta_\nu x^{(k+1)}+O(h^{k+2}).$$

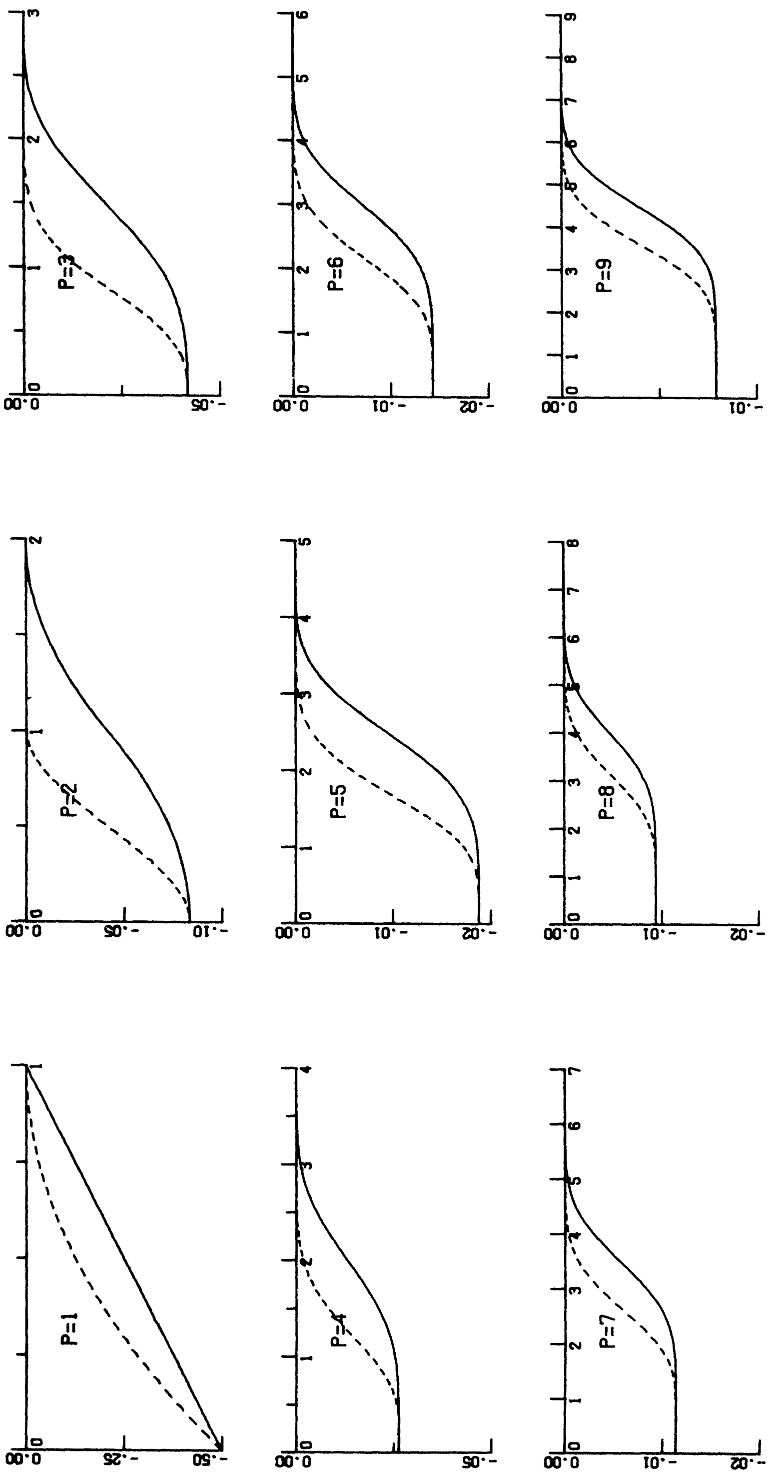


FIGURE 5

*The functions* $\gamma(t)$ *and* $C_{k+1}(\gamma(t) - \tilde{\gamma}(t))/(C_{k+1} - \tilde{C}_{k+1})$.

*Proof*. This theorem is an immediate consequence of Lemmas 2 and 4. □

We conclude this section with some interpretative remarks on Theorem 5. Ideally, one would like to see that Milne's device monitor the local discretization error

$$\delta_h(\mathscr{M}_{pc}, t) = h^{k+1}\left[C_{k+1}x^{(k+1)}(t) + \sum_\nu \gamma((t - s_\nu)/h)\Delta_\nu x^{(k+1)}\right] + O(h^{k+2}).$$

Instead, Milne's device monitors the quantity

$$h^{k+1}\left[C_{k+1}x^{(k+1)}(t) + \sum_\nu C_{k+1}\frac{\gamma((t - s_\nu)/h) - \tilde{\gamma}((t - s_\nu)/h)}{C_{k+1} - \tilde{C}_{k+1}}\Delta_\nu x^{(k+1)}\right] + O(h^{k+2}).$$

In Figure 5 we have plotted $\gamma(t)$ (dashed curve) and

$$C_{k+1}(\gamma(t) - \tilde{\gamma}(t))/(C_{k+1} - \tilde{C}_{k+1})$$

(solid curve).

It turns out that Milne's device does detect the jump in $x^{(k+1)}$, but one step later than it should. Therefore, assuming that the stepsize control mechanism is robust enough (and control mechanisms based on Milne's device usually are), we suggest the following strategy (also recommended by Gottwald and Wanner [10] for Rosenbrock methods): *If the control mechanism forces the stepsize to be decreased to integrate the FDE from $t_i$ to $t_i + h$, either because a previous attempt has been rejected or because of prudency (this may happen if the tolerance is approached closely), then reject the integration step from $t_{i-1}$ to $t_i$, and integrate from $t_{i-1}$ with decreased step.* In this way, the delayed detection of the jump may be used at the proper interval of integration. Note that this strategy does not require additional storage of $y(t_i)$ and $y'(t_i)$, since these values are stored for the calculation of the functional anyway.

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