Block Implicit One-Step Methods*

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Abstract. A class of one-step methods which obtain a block of r new values at each step are studied. The asymptotic behavior of both implicit and predictor-corrector procedures is examined.

1. Introduction. We shall consider a class of implicit one-step methods for solving ordinary differential equations which generalize the trapezoidal rule. The idea is to determine a block of r new values at each stage, the trapezoidal rule being a case with $r = 1$.

Implicit one-step methods have been studied by Stoller and Morrison [1], Ceschino and Kuntzmann [2] and Butcher [3]. For linear problems these methods are quite useful but with the exception of the trapezoidal rule they have not found favor for nonlinear problems because of the relatively great amount of work involved in advancing one step. Rosser [4] has suggested obtaining a block of new values simultaneously which makes the implicit methods more competitive. He discusses in detail a procedure which calculates four new values at each stage. In addition to his references to earlier work let us note the procedure of Clippinger and Dimsdale [5]—formula (3) cf. Section 2 below—which obtains two new values at each stage.

The methods we study can be described theoretically as block one-step methods. This situation prevails in practice for indefinite integrals and linear problems and also for general problems when we iterate to a fixed accuracy. In Section 2 we show convergence of these methods and study stability for a particular method. As Rosser indicates, one always expects good stability properties and indeed our example is a fourth order procedure which is A-stable.

For theoretical purposes the trapezoidal rule can be conveniently regarded as a one-step method but its practicality depends on computing with it as a predictor-corrector procedure. This is what we shall do in the general case. In Section 3 we shall show that a suitable predictor-corrector approach leads to the same asymptotic behavior as iterating to completion. Again we discuss the stability of an example.

Some comparative numerical examples are presented in Section 4.

2. Implicit Methods. We wish to approximate the solution of

$$u'(x) = f(x, u(x)), \qquad u(a) = s \tag{1}$$

on the interval $[a, b]$. Supposing f is continuous and satisfies

$$|f(x, y) - f(x, z)| \leqq L|y - z| \tag{2}$$

on $[a, b] \times (-\infty, \infty)$ guarantees the existence of a unique solution $u(x) \in C'[a, b]$.

Received October 22, 1968, revised March 3, 1969.

* This research was partially supported by the U. S. Atomic Energy Commission and by National Science Foundation grant 5967.

Rather than make specific differentiability assumptions, we shall assume u has continuous derivatives on $[a, b]$ of any order needed.

For $h \in (0, h_0]$ let $x_k = a + kh$. A sequence y_k which approximates $u(x_k)(= u_k$ below) is generated as follows. Let $y_0 = s$. An r-block method generates r additional terms simultaneously. After obtaining y_n for $n = mr$ the values $y_{n+1}, \cdots, y_{n+r}$ are to satisfy formulas of the form

$$\sum_{j=1}^{r} a_{ij} y_{n+j} = e_i y_n + h d_i f_n + h \sum_{j=1}^{r} b_{ij} f_{n+j}, \qquad i = 1, \cdots, r.$$

Here the a_{ij}, e_i, d_i, b_{ij} are constants and f_{n+j} denotes $f(x_{n+j}, y_{n+j})$.

For example, Clippinger and Dimsdale use

$$\begin{aligned} y_{n+1} - \frac{1}{2} y_{n+2} &= \frac{1}{2} y_n + \frac{h}{4} f_n - \frac{h}{4} f_{n+2}, \\ y_{n+2} &= y_n + \frac{h}{3} f_n + \frac{4h}{3} f_{n+1} + \frac{h}{3} f_{n+2}. \end{aligned} \tag{3}$$

Using vector notation and the matrices $\mathbf{A} = (a_{ij})$, $\mathbf{B} = (b_{ij})$, column vectors $\mathbf{e} = (e_1, \cdots, e_r)^T$, $\mathbf{d} = (d_1, \cdots, d_r)^T$, and $\mathbf{y}_m = (y_{n+1}, \cdots, y_{n+r})^T$, $\mathbf{F}(\mathbf{y}_m) = (f_{n+1}, \cdots, f_{n+r})^T$, this is

$$\mathbf{A}\mathbf{y}_m = h\mathbf{B}\mathbf{F}(\mathbf{y}_m) + \mathbf{e}y_n + h\mathbf{d}f_n.$$

For the practical use of such formulas we want to multiply through by $\mathbf{A}^{-1}$ which we suppose exists. Thus we may suppose $\mathbf{A} = \mathbf{I}$ and work with

$$\mathbf{y}_m = h\mathbf{B}\mathbf{F}(\mathbf{y}_m) + \mathbf{e}y_n + h\mathbf{d}f_n. \tag{4}$$

In this form the formulas (3) become

$$\mathbf{B} = \begin{pmatrix} 2/3 & -1/12 \\ 4/3 & 1/3 \end{pmatrix}, \qquad \mathbf{e} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \qquad \mathbf{d} = \begin{pmatrix} 5/12 \\ 1/3 \end{pmatrix}. \tag{5}$$

Since any reasonable method will integrate $f \equiv 0$ correctly we shall always require $\mathbf{e} = (1, 1, \cdots, 1)^T$ in (4).

To see when $\mathbf{y}_m$ is well defined by (4) let us consider the iterative procedure which starts with an arbitrary initial guess $\mathbf{y}_m^{(0)}$ and defines the sequence of iterates $\mathbf{y}_m^{(k)}$ by

$$\mathbf{y}_m^{(k+1)} = h\mathbf{B}\mathbf{F}(\mathbf{y}_m^{(k)}) + \mathbf{e}y_n + h\mathbf{d}f_n.$$

It is convenient to use the maximum norm

$$\|\mathbf{y}_m\| = \max_{1 \leq i \leq r} |y_{n+i}|$$

to discuss convergence of this process.

In this norm $\mathbf{F}$ satisfies a Lipschitz condition since each component does:

$$\|\mathbf{F}(\mathbf{w}) - \mathbf{F}(\mathbf{z})\| \leqq L\|\mathbf{w} - \mathbf{z}\|.$$

Obviously

$$\|\mathbf{y}_m^{(k+2)} - \mathbf{y}_m^{(k+1)}\| \leqq hL\|\mathbf{B}\| \, \|\mathbf{y}_m^{(k+1)} - \mathbf{y}_m^{(k)}\|.$$

If we require

$$h_0 L \|\mathbf{B}\| < 1 , \tag{6}$$

then a contraction mapping is present, the iterative procedure converges, and $\mathbf{y}_m$ is well defined as the unique solution of (4).

For the formula (5), $\|\mathbf{B}\| = 5/3$ and (6) is $h_0 L < 0.6$. This is rather more restrictive than is desirable though Rosser obtains satisfactory results with a formula requiring a more stringent condition. Intuitively one expects convergence to be slower for the component y_{n+2} than for y_{n+1}. The sufficient condition can be relaxed by using a weighted L_2 norm. For $d > 0$ let $\mathbf{D} = \operatorname{diag}\{1, d\}$ and use the new norm

$$\|\mathbf{y}_m\| = \|\mathbf{D}\mathbf{y}_m\|_2 .$$

A little computation shows the condition (6) becomes $h_0 L \|\mathbf{D}\mathbf{B}\mathbf{D}^{-1}\|_2 < 1$ and that it is best to use $d = 1/4$ which leads to the improved requirement $h_0 L < 1.27$.

In this section we are thinking of solving the implicit equations exactly or, like Rosser, iterating until they are resolved to a fixed accuracy. The equations are explicit in the case of indefinite integrals. In view of the remarkable stability we shall establish and the self-starting nature of the methods, they furnish a very effective scheme for such problems in comparison with the general scheme studied by Krylov [6]. Much the same can be said about linear problems when we solve the equation (5), which is now linear, exactly.

2.1. *Convergence.* For convenience we shall prove convergence in the maximum norm and accordingly suppose (6) holds in this norm. The discretization error $\boldsymbol{\varepsilon}_m$ is defined by

$$\mathbf{u}_m = h\mathbf{B}\mathbf{F}(\mathbf{u}_m) + \mathbf{e}u_n + h\mathbf{d}u'(x_n) + \boldsymbol{\varepsilon}_m \tag{7}$$

which is to hold for any smooth function $u(x)$, in particular a solution of (1) when $u'(x) = f(x, u(x))$. For example the formula (5) leads to

$$\boldsymbol{\varepsilon}_m = \left(\frac{h^4}{24} u^{(4)}(\zeta_{n+1}), -\frac{h^5}{90} u^{(5)}(\zeta_{n+2})\right)^T .$$

This is the most accurate formula possible of the form (4) with $r = 2$. Similarly the trapezoidal rule is the most accurate with $r = 1$.

It happens that advantage can be taken of formulas which are more accurate at the end of the block than in the middle as exemplified above. We shall prove (5) has global convergence like $O(h^4)$ instead of the $O(h^3)$ one might expect. Accordingly we suppose that there are γ_1, γ_2, k such that for all $n = mr$

$$\|\boldsymbol{\varepsilon}_m\| \leqq \gamma_1 h^k , \qquad |\epsilon_{n+r}| \leqq \gamma_2 h^{k+1} . \tag{8}$$

The procedure can be regarded as an implicit one-step method with step size rh for calculating y_n, y_{n+r}, $\cdots$. From (4)

$$\begin{aligned} y_{n+r} &= y_n + rh\left[\frac{1}{r} d_r f(y_n) + \frac{1}{r}\sum_{j=1}^{r} b_{rj} f(y_{n+j})\right] \\ &= y_n + rh\Phi(x_n, y_n; rh) . \end{aligned}$$

This is the same sort of procedure as used by Butcher [3], the distinction being that

our intermediate computations $y_{n+1}, \cdots, y_{n+r-1}$ are also used to represent the solution of the differential equation and not thrown away. Convergence of this one-step procedure is assured by Theorem 2.2 of Henrici [10], the only hypothesis not being obvious is the Lipschitz continuity of the second variable of the increment function. To see this we must first observe $\mathbf{y}_m$ depends Lipschitz continuously on y_n. For if

$$\mathbf{y}_m^* = h\mathbf{B}\mathbf{F}(\mathbf{y}_m^*) + \mathbf{e}y_n^* + h\mathbf{d}f(y_n^*) ,$$

then using (4)

$$\|\mathbf{y}_m - \mathbf{y}_m^*\| \leqq hL\|\mathbf{B}\| \, \|\mathbf{y}_m - \mathbf{y}_m^*\| + (1 + hL\|\mathbf{d}\|)|y_n - y_n^*|$$

hence

$$\|\mathbf{y}_m - \mathbf{y}_m^*\| \leqq \mathfrak{L}|y_n - y_n^*|$$

for suitable $\mathfrak{L}$ and all h less than the h_0 of (6). The same argument shows

$$\|\mathbf{y}_m - \mathbf{u}_m\| \leqq \mathfrak{L}|y_n - u_n| + \gamma_3 h^k . \tag{9}$$

Now

$$\begin{aligned} |\Phi(x, y_n; rh) - \Phi(x, y_n^*; rh)| &\leqq \frac{L}{r} [\|\mathbf{d}\| \, |y_n - y_n^*| + \|\mathbf{B}\| \, \|\mathbf{y}_m - \mathbf{y}_m^*\|] \\ &\leqq |y_n - y_n^*| \left[\frac{L}{r} (\|\mathbf{d}\| + \mathfrak{L}\|\mathbf{B}\|) \right] . \end{aligned}$$

We conclude from Henrici's theorem that there is a γ_4 such that for all x_n $(= a + nh = a + mrh) \leqq b$, $|y_n - u_n| \leqq \gamma_4 h^k$ which combined with (9) shows

$$\|\mathbf{y}_m - \mathbf{u}_m\| \leqq h^k(\mathfrak{L}\gamma_4 + \gamma_3) ;$$

this is the desired bound at all mesh-points. In particular if $u(x) \in C^5[a, b]$, the method (5) is convergent of $O(h^4)$.

2.2. *Stability.* As with the usual one-step methods our convergence proof shows there is no asymptotic stability problem. There are a number of ways of studying stability for fixed h, see [7, p. 191]. The main idea is to explicitly obtain the approximate solution y_k when the method is applied to

$$u'(x) = Au(x) , \qquad u(0) = s > 0 \tag{10}$$

with constant A and to require qualitative agreement with $u(x_k)$. Commonly y_k is obtained from a linear difference equation with constant coefficients in which A and h appear only as a product $\lambda = Ah$. When $\lambda < 0$, $u(x)$ decreases to zero and a method is said to be absolutely stable for $\lambda \in (-H, 0)$ if then y_k also decreases to zero. If H is the largest number for which this is true, it is called the stability boundary. More generally Dahlquist [8] allows complex A and calls a method A-stable if y_k tends to zero for all A with $\operatorname{Re} A < 0$. The notion of relative stability [9] is also popular but is quite inappropriate here since all these one-step methods are always trivially stable in this sense.

We shall study the stability of the scheme (5). The eigenvalues of $\mathbf{B}$ are $\mu = (3 \pm i\sqrt{3})/6$. If $\lambda \neq 1/\mu$, one easily finds that applying (5) to (10) gives

$$y_{n+1} = \frac{6 - \lambda^2}{6 - 6\lambda + 2\lambda^2} y_n \equiv S(\lambda) y_n ,$$

$$y_{n+2} = \frac{3 + 3\lambda + \lambda^2}{3 - 3\lambda + \lambda^2} y_n \equiv R(\lambda) y_n .$$

Accordingly

$$y_{2m} = R(\lambda)^m y_0 , \qquad y_{2m+1} = S(\lambda) R(\lambda)^m y_0 .$$

Clearly if we fix h, the discrete solution tends to zero if and only if $|R(\lambda)| < 1$. A simple computation shows this is the case for all λ with Re $(\lambda) < 0$. Thus the method is A-stable. We remark that Dahlquist proves that of the linear multistep methods the trapezoidal rule is the most accurate A-stable method.

3. Predictor-Corrector Methods. For nonlinear problems we do not ordinarily proceed as in Section 2. Rather than iterate until (2.4) is satisfied, we only iterate a fixed number of times. Since a good guess for $\mathbf{y}_m$ is required we use the data computed in the previous block to predict $\mathbf{y}_m$ via explicit formulas. Of course, in the first block we can predict $y_k = y_0 + khf_0$ and iterate to completion. This is the normal usage for the trapezoidal rule but there seems to be very little of such usage for block and implicit methods. Clippinger and Dimsdale do use their formula in this way and Rosser also points out this possibility. To our way of thinking it is precisely this procedure that makes block implicit methods practical. Indeed the procedure we describe uses only two function evaluations per step just as do the usual predictor-corrector methods. We gain the advantages of self-starting and easy change of step-size.

3.1. *Asymptotic Behavior.* We shall prove that a suitable predictor-corrector scheme asymptotically gives the same result as iterating to completion. Recall that the values obtained by iterating to completion satisfy

$$\mathbf{y}_m = h\mathbf{B}\mathbf{F}(\mathbf{y}_m) + \mathbf{e}y_n + h\mathbf{d}f(y_n) \tag{1}$$

and $\mathbf{y}_m = \mathbf{u}_m + O(h^k)$ ($\mathbf{u}_m$ is the solution of the differential equation). In the predictor-corrector scheme we suppose that the first block is obtained by iterating to completion; other starting procedures are easily handled by our analysis.

Following the suggestion of [9] we predict new values in a block $\mathbf{y}_m{}^P$, evaluate $\mathbf{F}(\mathbf{y}_m{}^P)$, correct to obtain $\mathbf{y}_m{}^c$, evaluate $\mathbf{F}(\mathbf{y}_m{}^c)$, and correct again to obtain $\mathbf{y}_m{}^{cc}$. The values of $\mathbf{F}(\mathbf{y}_m{}^c)$ and $\mathbf{y}_m{}^{cc}$ are accepted; this is the P(EC)^2 method. It is perhaps more common to accept $\mathbf{F}(\mathbf{y}_m{}^c)$ and $\mathbf{y}_m{}^c$ (PECE), however this procedure costs exactly the same—two function evaluations per step—and is in some respects desirable. The method of proof we give shows the PECE mode has the same order of convergence as iterating to completion but not that they have the same asymptotic behavior. Indeed, this is probably not true in general. The method does show P(EC)^2 and other procedures with more function evaluations to have the same asymptotic behavior. For this reason we give details for the P(EC)^2 mode although PECE is the more stable.

We define $\mathbf{y}_0 = \mathbf{y}_0{}^c = \mathbf{y}_0{}^{cc}$ which is consistent with our starting procedure. We shall use a predictor of the form

$$\mathbf{y}_m^{\,p} = \mathbf{M}\mathbf{y}_{m-1}^{cc} + h\mathbf{N}\mathbf{F}(\mathbf{y}_{m-1}^{c}) + \mathbf{p}y_{n-r}^{cc} + h\mathbf{q}f(y_{n-r}^{c}) \,. \tag{2}$$

Using $\mathbf{y}_m{}^p$ we form a corrected value $\mathbf{y}_m{}^c$ by

$$\mathbf{y}_m{}^c = h\mathbf{B}\mathbf{F}(\mathbf{y}_m{}^p) + \mathbf{e}y_n{}^{cc} + h\mathbf{d}f(y_n{}^c) \tag{3}$$

and a second corrected value

$$\mathbf{y}_m{}^{cc} = h\mathbf{B}\mathbf{F}(\mathbf{y}_m{}^c) + \mathbf{e}y_n{}^{cc} + h\mathbf{d}f(y_n{}^c) \,. \tag{4}$$

It is quite easy to show $\mathbf{y}_m{}^{cc} = \mathbf{u}_m + O(h^k)$ so that the predictor-corrector procedure is convergent at the same rate as iterating to completion. However, to show the procedures have the same asymptotic behavior we have to show $\mathbf{y}_m{}^{cc} = \mathbf{y}_m + O(h^{k+1})$ which implies the error terms of $O(h^k)$ are identical.

If we define $\|\mathbf{y}_{-1} - \mathbf{y}_{-1}^{cc}\| = \|\mathbf{y}_{-1} - \mathbf{y}_{-1}\| = 0$, then (1), (3), (4) imply

$$\|\mathbf{y}_m - \mathbf{y}_m{}^c\| \leqq hL\|\mathbf{B}\| \, \|\mathbf{y}_m - \mathbf{y}_m{}^p\| + \|\mathbf{y}_{m-1} - \mathbf{y}_{m-1}^{cc}\| + hL\|\mathbf{d}\| \, \|\mathbf{y}_{m-1} - \mathbf{y}_{m-1}^{c}\| \,, \tag{5}$$

$$\|\mathbf{y}_m - \mathbf{y}_m{}^{cc}\| \leqq hL\|\mathbf{B}\| \, \|\mathbf{y}_m - \mathbf{y}_m{}^c\| + \|\mathbf{y}_{m-1} - \mathbf{y}_{m-1}^{cc}\| + hL\|\mathbf{d}\| \, \|\mathbf{y}_{m-1} - \mathbf{y}_{m-1}^{c}\| \,. \tag{6}$$

We suppose that for any smooth function $u(x)$

$$\mathbf{u}_m = \mathbf{M}\mathbf{u}_{m-1} + h\mathbf{N}\mathbf{F}(\mathbf{u}_{m-1}) + \mathbf{p}u_{n-r} + h\mathbf{q}f(u_{n-r}) + \boldsymbol{\delta}_m$$

where $\boldsymbol{\delta}_m = O(h^k)$. Taking $u(x)$ to be the solution of the differential equation and using $\mathbf{y}_m = \mathbf{u}_m + O(h^k)$ and (2), we find

$$\begin{aligned} \|\mathbf{y}_m - \mathbf{y}_m{}^p\| \leqq{}& \|\mathbf{M}\| \, \|\mathbf{y}_{m-1} - \mathbf{y}_{m-1}^{cc}\| + \|\mathbf{p}\| \, \|\mathbf{y}_{m-2} - \mathbf{y}_{m-2}^{cc}\| \\ &+ hL\|\mathbf{N}\| \, \|\mathbf{y}_{m-1} - \mathbf{y}_{m-1}^{c}\| + hL\|\mathbf{q}\| \, \|\mathbf{y}_{m-2} - \mathbf{y}_{m-2}^{c}\| + \gamma h^k \end{aligned} \tag{7}$$

for suitable constant $\gamma \geqq 0$.

For constants $\alpha > 1$, $\beta > L\|\mathbf{B}\|\gamma$, $\delta = L\|\mathbf{d}\| + L\|\mathbf{B}\|$ we define the sequence e_m by $e_{-1} = 0$,

$$e_m = e_{m-1}[1 + h\alpha\delta] + \beta\delta h^{k+2} \,, \qquad m = 0, 1, \cdots \,.$$

We claim that for all sufficiently small h and all $m = 0, 1, \cdots$

$$\|\mathbf{y}_m - \mathbf{y}_m^{c}\| \leqq \alpha e_{m-1} + \beta h^{k+1} \,, \qquad \|\mathbf{y}_m - \mathbf{y}_m{}^{cc}\| \leqq e_m \,. \tag{8}$$

This is obviously true for $m = 0$. Suppose it is true for all indices through $m - 1$. Noting that e_m is increasing in m, the induction assumption and (7) imply there are constants C_1, C_2 such that for all sufficiently small h

$$\|\mathbf{y}_m - \mathbf{y}_m{}^p\| \leqq C_1 e_{m-1} + \gamma h^k + C_2 h^{k+2} \,.$$

Using this and (5) we find there are constants C_3, C_4 such that

$$\|\mathbf{y}_m - \mathbf{y}_m{}^c\| \leqq e_{m-1}(1 + hC_3) + L\|\mathbf{B}\|\gamma h^{k+1} + C_4 h^{k+2} \leqq \alpha e_{m-1} + \beta h^{k+1} \,,$$

the last inequality holding for all sufficiently small h because of the conditions on α, β. This result, the induction assumption, and (6) yield

$$\|\mathbf{y}_m - \mathbf{y}_m{}^{cc}\| \leqq e_{m-1}[1 + h\alpha(L\|\mathbf{B}\| + L\|\mathbf{d}\|)] + \beta(L\|\mathbf{B}\| + L\|\mathbf{d}\|)h^{k+2} = e_m \,.$$

Thus our claim is true by induction.

A standard argument [10, p. 18] shows that for $mrh \leqq b - a$,

$$e_m \leqq \beta h^{k+1} e^{\alpha\delta(b-a)}(1/\alpha + \delta h) \,.$$

Together with (8) this says $\mathbf{y}_m{}^{cc} = \mathbf{y}_m + O(h^{k+1})$ uniformly on $[a, b]$ which is the desired conclusion.

3.2. *Stability.* In contrast to the situation of subsection 2.2, stability for finite h appears to be the most serious limitation of block implicit methods when used as a predictor-corrector combination of the type suggested. We shall study the Clippinger-Dimsdale formula and obtain its stability boundary for a number of procedures. By way of comparison we recall that the stability boundary is

2.785 for the fourth-order Runge-Kutta,
1.285 Adams-Moulton, Adams-Bashforth PECE,
1.000 Stabilized Milne.

We only study predictors which use y and y' values as in the analysis of the previous section. Thus as in (2) the form is exemplified by

$$y_{n+1}^p = c_{21}y_{n-2} + c_{22}y_{n-1} + c_{23}y_n + h(d_{21}y'_{n-2} + d_{22}y'_{n-1} + d_{23}y_n') .$$

Predictors of orders four, five and six which minimize

$$\sum c_{ik}^2 \quad \text{and} \quad \sum c_{ik}^2 + \sum d_{ik}^2$$

were examined. These quantities affect the propagation of uncorrelated noise and it was felt their minimization would lead to reasonable formulas. Formulas of orders six and five have no and one free parameter respectively and yield unsatisfactory formulas. The two fourth-order formulas differ little; the simpler set is

$$\begin{aligned} y_{n+1}^p &= \frac{1}{3}(y_{n-2} + y_{n-1} + y_n) + \frac{h}{6}(3y'_{n-2} - 4y'_{n-1} + 13y_n') , \\ y_{n+2}^p &= \frac{1}{3}(y_{n-2} + y_{n-1} + y_n) + \frac{h}{12}(29y'_{n-2} - 72y'_{n-1} + 79y_n') . \end{aligned} \tag{9}$$

It is a little simpler to determine the stability boundary of $\mathrm{PE(CE)}^k$ modes than for $\mathrm{P(EC)}^2$ so we shall just give details for them. It is convenient now to define the vectors for $n = mr$,

$$\begin{aligned} \mathbf{Y}_0{}^{cc} &= (y_0, y_1, y_2)^T , \\ \mathbf{Y}_m{}^{p} &= (y_n{}^{cc}, y_{n+1}^p, y_{n+2}^p)^T , \\ \mathbf{Y}_m{}^{c} &= (y_n{}^{cc}, y_{n+1}^c, y_{n+2}^c)^T , \\ \mathbf{Y}_m{}^{cc} &= (y_n{}^{cc}, y_{n+1}^{cc}, y_{n+2}^{cc})^T . \end{aligned}$$

Now if we use the matrices

$$\mathbf{C} = \begin{pmatrix} 0 & 0 & 1 \\ c_{21} & c_{22} & c_{23} \\ c_{31} & c_{32} & c_{33} \end{pmatrix}, \qquad \mathbf{D} = \begin{pmatrix} 0 & 0 & 0 \\ d_{21} & d_{22} & d_{23} \\ d_{31} & d_{32} & d_{33} \end{pmatrix},$$

$$\mathbf{P} = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \qquad \mathbf{Q} = \begin{pmatrix} 0 & 0 & 0 \\ 5/12 & 2/3 & -1/12 \\ 1/3 & 4/3 & 1/3 \end{pmatrix},$$

then

$$\mathbf{Y}_{m+1}^{p} = (\mathbf{C} + \lambda\mathbf{D})\mathbf{Y}_{m}^{cc},$$
$$\mathbf{Y}_{m+1}^{c} = (\mathbf{P} + \lambda\mathbf{Q})\mathbf{Y}_{m+1}^{p},$$
$$\mathbf{Y}_{m+1}^{cc} = (\mathbf{P} + \lambda\mathbf{Q})\mathbf{Y}_{m+1}^{c} = (\mathbf{P} + \lambda\mathbf{Q})^{2}(\mathbf{C} + \lambda\mathbf{D})\mathbf{Y}_{m}^{cc}.$$

In general for PE(CE)^k

$$\mathbf{Y}_{m+1}^{(k)} = (\mathbf{P} + \lambda\mathbf{Q})^{k}(\mathbf{C} + \lambda\mathbf{D})\mathbf{Y}_{m}^{(k)}$$

which implies $\mathbf{Y}_{m}^{(k)} = \mathbf{T}^{m}\mathbf{Y}_{0}^{(k)}$ where $\mathbf{T} = (\mathbf{P} + \lambda\mathbf{Q})^{k}(\mathbf{C} + \lambda\mathbf{D})$. From this representation we see that the stability boundary is the largest number H such that if $\lambda \in (-H, 0)$, then all the eigenvalues of $\mathbf{T}$ have modulus less than one. For the predictors (9) we have found for PE(CE)^k

k	1	2	3	4
H	0.439	0.694	0.934	1.293

A similar analysis shows $H = 0.410$ for the P(EC)^2 mode.

4. Numerical Results. In this section we compare numerically our example and several well-known and widely used fourth-order schemes. The methods are:

RK: Runge-Kutta scheme with classical parameters.

ABM: Adams-Bashforth, Adams-Moulton PECE scheme.

SM: Stabilized Milne method as described in Stetter's paper [11].

BOS: Predictor-corrector mode of the block one-step method using (3.9).

BOSLS: Block one-step method (as applied to linear problems) with the corrector pair of equations being solved exactly using a Gaussian elimination routine.

Because of the stability limitation of the particular BOS scheme above and because more promising approaches for predictors are currently being investigated, only a limited comparison of the above methods was undertaken. The sample problem set consisted of ten linear and ten nonlinear first-order differential equations.

The problem of Table 1 is

$$y'(x) = -y(x), \quad y(0) = 1, \qquad 0 \leqq x \leqq 20, \quad h = 0.25.$$

The problem of Table 2 is

$$y'(x) = -y^{2}(x), \quad y(0) = 1, \qquad 0 \leqq x \leqq 20, \quad h = 2^{-5}.$$

The results for both linear and nonlinear problems were generally consistent and indicated that BOS and BOSLS (where applicable) are competitive with the other methods. For h near the stability boundary, BOS naturally does not yield acceptable answers. However, for h small enough that the computed solution is correct to nearly machine accuracy, BOS generally produced the smallest relative errors. For intermediate values of h, it was frequently the case that BOS produced more accurate results than RK and ABM but less accurate than SM, with BOS and BOSLS being essentially equivalent. For small h, BOSLS was less accurate than

BOS, a factor attributed to the inaccuracies of the represented linear system as $h \to 0$ and the resulting numerical inversion. On the other hand, BOSLS is stable for all h and, in fact, yields a solution correct to machine accuracy for the problem $y' = 100(y - x)$, $y(0) = 0.1$ with $h = 1/2$. None of the other methods were capable of computing a stable solution for any reasonable h. The two examples of Tables 1, 2 are representative of the results from the whole sample problem set.

The starting procedure supplies each routine with the necessary number of exact values prior to the initial starting point. In this way, the first computed solution value occurs at $x_0 + h$ for all the methods. Also, except for the starting procedure, the comparisons are based on an equal number of function evaluations for the fixed interval of integration. Thus the stepsize for the RK method is $2h$. The tabulated values are the relative discretization errors $(y_n - u(x_n))/u(x_n)$. All computations were performed on a CDC 3600.

TABLE 1. *Linear Problem. Relative Error* $\times 10^{-3}$

x	BOSLS	BOS	SM	RK	ABM
2	0.18	− 2.4	0.26	1.6	− .70
4	0.35	− 7.5	0.52	3.2	−1.4
6	0.53	−13	0.77	4.8	−2.1
8	0.71	−20	1.0	6.4	−2.8
10	0.88	−26	1.3	7.9	−3.5
12	1.1	−33	1.5	9.5	−4.2
14	1.2	−39	1.8	11	−4.9
16	1.4	−45	2.0	13	−5.6
18	1.6	−52	2.3	14	−6.3
20	1.8	−58	2.5	16	−7.0

TABLE 2. *Nonlinear Problem. Relative Error* $\times 10^{-8}$

x	BOS	SM	RK	ABM
2	−6.7	7.2	6.8	−47
4	−4.0	4.4	4.2	−29
6	−2.8	3.2	3.0	−21
8	−2.2	2.5	2.3	−16
10	−1.8	2.0	1.9	−13
12	−1.5	1.7	1.6	−11
14	−1.3	1.5	1.4	− 9.7
16	−1.2	1.3	1.2	− 8.5
18	−1.0	1.2	1.1	− 7.6
20	−0.94	1.1	0.99	− 6.9

5. Remarks. It is a trivial matter to alter our analysis so as to permit unequal spacing within a block. As long as the mesh-points are reasonably close to even spacing we may rightfully claim r new computed values per block. This remark is important if one considers formulas with $r = 3$ for only convergence of order four may be obtained with evenly spaced points. By spacing so that the quadrature formula for y_{n+3} is the appropriate Lobatto formula, a fifth-order procedure is obtained with a spacing quite acceptably even.

The stability of the predictor-corrector methods appears to be their most serious disadvantage. There are other ways of organizing the computations with the predictors which seem to improve the stability a great deal. We have generated a suitable procedure with the correctors (2.5) which at a cost of two function evaluations per step has an experimentally determined stability boundary greater than 1. We are currently investigating this promising approach.

Portions of this paper have been much improved because of constructive criticism by an anonymous referee.

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