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1. Introduction

Many physical systems are described by ordinary differential equations whose solutions contain time constants differing greatly in magnitude. Such equations are called stiff. When a classical numerical integration procedure is applied to a stiff system of equations, the step size is generally determined by the component of the solution with the largest decay rate, while the region of integration is determined by the component with the smallest rate. After the initial transient, the rapidly decaying components are insignificant, but the step size must remain small to prevent numerical instability. As a result, the time required to integrate a highly stiff system can become excessive.

A-stable methods are often used to overcome this problem because the step size of an A-stable method is governed only by the allowable discretization error. The step size for A-stable linear multistep methods must remain small, however, because the order of such methods cannot exceed two. Implicit one-step methods are free from this restriction on order, and several classes of A-stable implicit one-step methods of arbitrary order exist. Unfortunately, these implicit methods are relatively inefficient. Their efficiency can be improved, however, by obtaining a block of new values simultaneously. These block implicit one-step methods have been studied by Rosser [7] and Shampine and Watts [8]. We present in this paper a new class of block implicit methods possessing desirable stability properties.

We shall restrict our discussion to a single equation for simplicity. The generalization to systems of equations will be obvious. We first describe general block implicit methods and our new class of methods. We then present a convergence theorem for general block implicit methods. Finally we discuss the stability of our methods.

2. Block Implicit Methods

We wish to approximate the solution of

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

on the interval $[a,b]$. Rather than make specific differentiability assumptions, we shall assume y has continuous derivatives on $[a,b]$ of any order required.

Let $x_n = a + nh$ for $n = 0, 1, \ldots$ and $h > 0$. We wish to generate a sequence $\{y_n\}$ which approximates the sequence of exact values $\{y(x_n)\}$. Let $y_0 = \alpha$. An s-block method generates a block of s additional terms simultaneously and ultimately produces values for all $n \in I_h$, where $I_h = \{n\colon 0 \le n \le ms\}$ and $m = [(b-a)/sh]$. Each block of values $\underset{\sim}{y}_\ell = (y_{n+1},\ldots,y_{n+s})^T$, where $n = \ell s$, satisfies equations of the form

$$y_{n+i} = y_n + h\sum_{j=1}^{i}\varphi_j(x_n,y_n,\ldots,y_{n+s},h), \quad i = 1, \ldots, s. \tag{2}$$

The increment functions φ_j are determined by f and are functions of x_n, y_n, $\ldots$, y_{n+s}, and h only. We shall assume they are defined in the region R of $(x,\underset{\sim}{z},h)$ space defined by $x \in [a,b-sh]$, $z_k \in (-\infty,\infty)$,

$k = 0, \ldots, s$, and $h \in [0,h_0]$, where $h_0 < (b-a)/s$. The local discretization errors are defined by

$$d_i(x_n,h) = h\varphi_i(x_n,y(x_n),\ldots,y(x_{n+s}),h) - (y(x_{n+i}) - y(x_{n+i-1})),$$
$$i = 1, \ldots, s, \qquad (3)$$

and the order of the method is defined to be the largest integer r such that

$$|d_i(x,h)| = O(h^{r+1}), \quad i = 1, \ldots, s, \qquad (4)$$

in the region S of (x,h) space defined by $x \in [a,b-sh]$ and $h \in [0,h_0]$.

We propose s-block methods where each increment function is an interpolatory quadrature formula employing function values and possibly derivatives at nodes in the interval $[x_n,x_{n+s}]$, and values of y at nonmesh points are obtained from the Hermite interpolation polynomial interpolating the first $p_i - 1$ derivatives of y at x_{n+i} for $i = 0, \ldots, s$. Each such method can be written in the form

$$y_{n+i} = y_n + h\sum_{j=1}^{i} \sum_{k,\ell} w_{jk\ell} h^{\ell} f^{(\ell)}(x_{n+\theta},y_{n+\theta}), \quad i = 1, \ldots, s, \qquad (5)$$

where $\theta(j,k) \in [0,s]$, and

$$y_{n+\theta} = \sum_{i=0}^{s} \sum_{j=0}^{p_i-1} h^j \psi_{ij}(\theta) y_{n+i}^{(j)}. \qquad (6)$$

If each increment function has a degree of precision at least $q - 1$, then the method has order $r = \min[p,q]$, where $p = \Sigma\, p_i$.

3. Convergence

The following theorem gives sufficient conditions for the convergence of an s-block method and indicates the order of the accumulated discretization error. Our methods satisfy these conditions and hence are convergent.

THEOREM. Let there exist positive constants L, M, and r such that

$$|\varphi_i(x,\underset{\sim}{z},h) - \varphi_i(x,\underset{\sim}{z}^*,h)| \le L \sum_{j=0}^{s} |z_j - z_j^*|, \quad i = 1, \ldots, s, \tag{7}$$

for $(x,\underset{\sim}{z},h)$ and $(x,\underset{\sim}{z}^*,h) \in R$, and

$$|d_i(x,h)| \le Mh^{r+1}, \quad i = 1, \ldots, s, \tag{8}$$

for $(x,h) \in S$. Then for any $h < \min[h_0, 2/s(s+1)L]$, the difference equations (2) have a unique solution $\{y_n\}$, defined on I_h, and there is a constant N such that

$$|y_n - y(x_n)| \le Nh^r, \quad n \in I_h.$$

Proof. Suppose a partial solution satisfying the difference equations (2) has been found on the set $\{0,1,\ldots,n\}$, where $n = \ell s$ and $\ell < m$. Equations (2) can be written in the form $\underset{\sim}{y}_\ell = \underset{\sim}{\psi}(\underset{\sim}{y}_\ell)$, where

$$\psi_i(\underset{\sim}{y}) = y_n + h \sum_{j=1}^{i} \varphi_j(x_n, y_n, \underset{\sim}{y}, h), \quad i = 1, \ldots, s.$$

For arbitrary $\underset{\sim}{y}$ and $\underset{\sim}{y}^*$, the Lipschitz condition (7) implies that

$$\|\psi(y) - \psi(y^*)\|_1 \le \sum_{i=1}^{s} ihL\|y-y^*\|_1 = \lambda\|y-y^*\|_1,$$

where $\lambda = s(s+1)hL/2 < 1$. Hence ψ is a contraction mapping. Since ψ is defined for all y, it follows that equations (2) have a unique solution y_ℓ. Thus the partial solution can be continued uniquely throughout the set I_h.

A standard argument [5, p. 12] shows that the errors $e_n = |y_n - y(x_n)|$ satisfy

$$e_{\ell s+i} \le e_{\ell s} + ihL \sum_{j=0}^{s} e_{\ell s+j} + iMh^{r+1}, \quad i = 1, \ldots, s; \ \ell = 0, \ldots, m-1.$$

These relations can be written in the form $Ae_\ell \le b_\ell$ for $\ell = 0, \ldots, m-1$, where A and b_ℓ have elements

$$a_{ij} = \delta_{ij} - ihL, \quad i, j = 1, \ldots, s,$$

$$b_i = (1+ihL)e_{\ell s} + iMh^{r+1}, \quad i = 1, \ldots, s.$$

The inverse matrix A^{-1} has the elements

$$c_{ij} = ((1-s(s+1)hL/2)\delta_{ij} + ihL)/(1-s(s+1)hL/2), \quad i, j = 1, \ldots, s.$$

Since $A^{-1} \ge 0$, it follows that $e_\ell \le A^{-1}b_\ell$ for $\ell = 0, \ldots, m-1$. Define $\varepsilon_\ell = A^{-1}b_\ell$ for $\ell = 0, \ldots, m-1$, and set $\varepsilon_0 = 0$. The ε_n form a non-decreasing sequence and

$$\varepsilon_{(\ell+1)s} \le (1+shL^*)\varepsilon_{\ell s} + M^*h^{r+1}, \quad \ell = 0, \ldots, m-1,$$

for certain constants L^* and M^*. Another standard argument [5, p. 12] shows

$$\epsilon_{\ell s} \leq (M^* h^r / sL^*)(e^{L^*(b-a)} - 1), \quad \ell = 0, \ldots, m.$$

Since $e_n \leq \epsilon_n$ for $n \in I_h$, the desired result follows.

4. Stability

We shall examine the stability of our methods by applying them to the differential equation $y' = \lambda y$, where λ is a complex constant with $\mathrm{Re}(\lambda) < 0$. The method (5) can be interpreted as an implicit one-step method with step size sh. Substituting $y' = \lambda y$ in equations (5) and (6), we obtain

$$y_{n+s} = R(sh\lambda)y_n, \tag{9}$$

where $R(\mu)$ is a rational approximation to e^{μ}. Since R is a function of only the degrees of precision of the increment functions and the orders of collocation p_i of the Hermite interpolation polynomial, the stability of entire classes of methods can be analyzed simultaneously. Let $(p_0, \ldots, p_s)$ denote the class of methods of the form (5) whose increment functions have degrees of precision at least $\Sigma p_i - 1$. We shall characterize the stability of such classes in terms of the following concepts.

Definition. The class $(p_0, \ldots, p_s)$ is A-stable if $|R(\mu)| < 1$ for $\mathrm{Re}(\mu) < 0$.

Definition. The class $(p_0, \ldots, p_s)$ is stiffly stable if $|R(\mu)| < 1$ in the regions $\{\mu : \mathrm{Re}(\mu) \leq D\}$ and $\{\mu : D < \mathrm{Re}(\mu) < a, |\mathrm{Im}(\mu)| < \theta\}$.

Definition. The class $(p_0,\ldots,p_s)$ is strongly A- or strongly stiffly stable if it is A- or stiffly stable and $|R(\mu)| \to 0$ as $\mathrm{Re}(\mu) \to -\infty$.

We first consider the class (p,q) of 1-block methods employing higher derivatives.

THEOREM. Let $E_{ij}(\mu)$ denote the (i,j) entry in the Pade table for e^{μ}. Then $R(\mu) = E_{pq}(\mu)$ for the class (p,q).

Proof. A simple calculation shows that

$$R(\mu) = P_p(\mu)/Q_q(\mu),$$

where $P_p(\mu)$ and $Q_q(\mu)$ are polynomials of order p and q in μ. Since $R(\mu)$ must be an approximation to e^{μ} of order $p + q$, it follows that $R(\mu)$ must be the (p,q) entry in the Pade table for e^{μ}.

COROLLARY. Class (p,p) is A-stable and classes (p,p+1) and (p,p+2) are strongly A-stable for $p \geq 1$.

Proof. $|E_{ij}(\mu)| < 1$ for $\mathrm{Re}(\mu) < 0$ for $i = j \geq 0$ [1], $i = j-1 \geq 0$, and $i = j-2 \geq 0$ [4]. Finally, it is obvious that $|E_{ij}(\mu)| \to 0$ as $\mathrm{Re}(\mu) \to -\infty$ for $i < j$.

There are implicit one-step methods possessing similar stability properties. These include the method of Hermite [6]

$$y_{n+1} = y_n + \sum_{i=1}^{p} h^i \alpha_{pi} y_n^{(i)} - \sum_{i=1}^{q} h^i \beta_{qi} y_{n+1}^{(i)}, \tag{10}$$

where α_{pi} and β_{qi} are the ith coefficients in the numerator and denominator of E_{pq}, and the implicit Runge-Kutta processes developed by Butcher [2], Ehle [4], and Chipman [3]. However, the methods in the class (p,q) enjoy certain advantages. They attain the same order of accuracy as the scheme (10) while employing derivatives of lower order, and, unlike the Runge-Kutta processes, they require the solution of only one nonlinear equation at each time step.

We turn now to 2- and 3-block methods. Consider the class (p,p,p). It can be shown that

$$R(\mu) = P_{2p}(\mu)/P_{2p}(-\mu),$$

where $P_{2p}(\mu)$ is a polynomial of order 2p in μ. It follows that $|R(i\omega)| = 1$ for $\omega \in (-\infty,\infty)$ and $|R(\mu)| \to 1$ as $|\mu| \to \infty$ for all $p \geq 1$. Using the Routh-Hurwitz conditions, we have verified that $R(\mu)$ is regular for $\mathrm{Re}(\mu) < 0$ and hence that (p,p,p) is A-stable for p = 1, 2, and 3. We conjecture that this is true for all $p \geq 1$.

There are strongly A-stable and strongly stiffly stable 2- and 3-block methods. For example, the class (1,1,2) is strongly A-stable, and the classes (1,1,3), (1,2,2), (1,2,3), (2,2,3), (1,1,1,2), and (1,1,2,2) are strongly stiffly stable. Figure 1 shows the loci in the $h\lambda$ plane where $|R| = 1$ for these classes of methods. Since the loci are symmetric with respect to the real axis, only half of each locus is plotted. The regions of stability lie to the left of the loci. The regions of instability in the left half-plane are remarkably small. The corresponding regions for Gear's [5] stiffly stable linear multistep methods are larger by several orders of magnitude.

5. Concluding Remarks

We have presented a new class of block implicit one-step methods possessing desirable stability properties. Since they are implicit, their implementation is nontrivial and requires the development of effective and convergent iterative procedures and practical error estimation schemes. These problems are being studied and will be discussed elsewhere.

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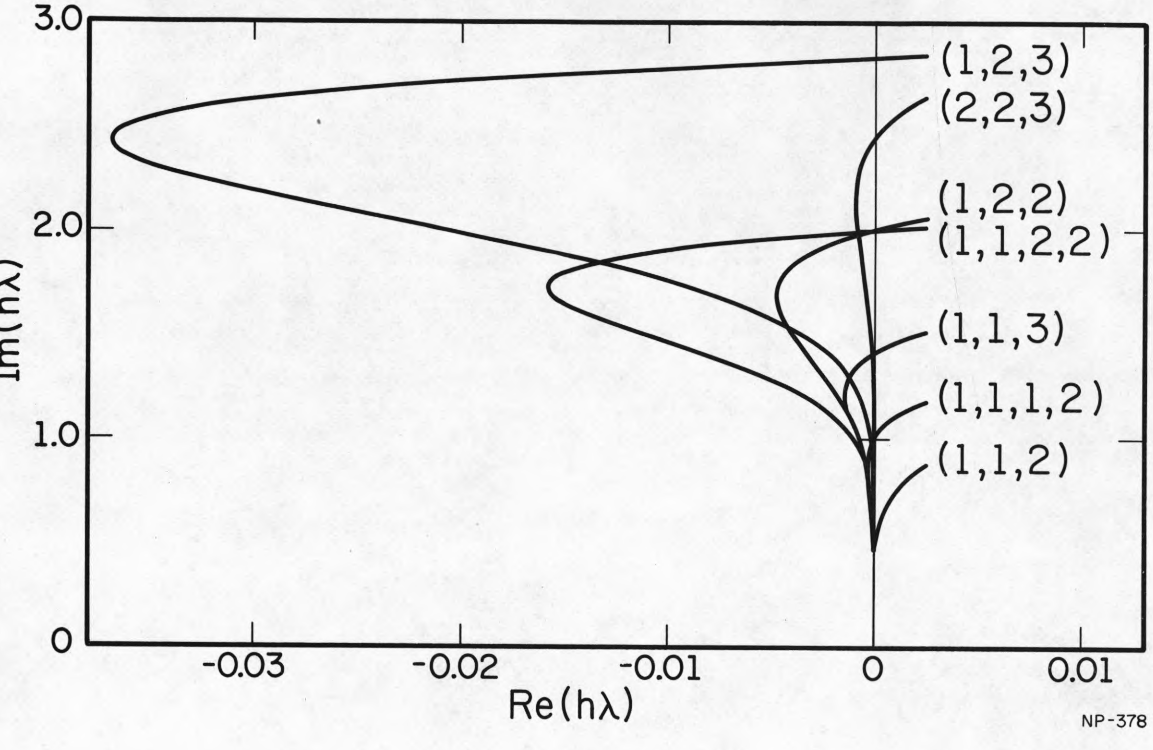

Figure 1. Stability regions for 2- and 3-block methods.

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13. ABSTRACT

A new class of block implicit one-step methods for ordinary differential equations is presented. The methods are based on quadrature and generate function values at nonmesh quadrature points through Hermite interpolation. A general convergence theorem for block implicit methods is proved, and the stability of the new class of methods is analyzed. The class is shown to contain A-stable, stiffly stable, strongly A-stable, and strongly stiffly stable methods.

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