A-STABLE AND L-STABLE BLOCK IMPLICIT ONE-STEP METHODS*

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Abstract

A class of methods for solving the initial problem for ordinary differential equations are studied. We develop k-block implicit one-step methods whose nodes in a block are nonequidistant. When the components of the node vector are related to the zeros of Jacobi's orthogonal polynomials $P_{k-1}^{(1,1)}(u)$ or $P_{k-1}^{(1,0)}(u)$, we can derive a subclass of formulas which are A- or L-stable. The order can be arbitrarily high with A- or L-stability. We suggest a modified algorithm which avoids the inversion of a $km\times km$ matrix during Newton-Raphson iterations, where m is the number of differential equations. When $k=4$, for example, only a couple of $m\times m$ matrices have to be inversed, but four values can be obtained at one time.

§ 1. Introduction

We shall study a class of methods for solving numerically the initial value problem for ordinary differential equations. These procedures, termed k-block implicit one-step methods, advance the numerical solution by a block of k new solution values at one time. The nodes of a block can be nonequidistant.

Because implicit one-step methods have many merits, such as self-starting, easy change of steplength, high accuracy and good stability, they have attracted much attention from a number of authors, e.g., Butcher[3,4], Shampine and Watts[10,11], Williams and Frand de Hoog[12] and Bichart and Picel[1]. However, the block methods with nonequidistant nodes have not received as much attention. Shampine and Watts[10,11] presented a different approach based on interpolatory formulas of Newton-Cotes type, whose block methods for sizes $k=1, 2, \cdots, 8$ are A-stable, but for $k=9$, 10 are not. Bichart and Picel[1] also had a detailed study of block implicit methods which are stiffly stable at least through order 25.

In this paper, we continue the study of general k-block implicit methods with nonequidistant nodes. The formulas developed by Shampine and Watts[11] are involved. If the components of a node vector are related to the zeros of Jacobi's orthogonal polynomials $P_{k-1}^{(1,1)}(u)$ or $P_{k-1}^{(1,0)}(u)$, we can derive a subclass of formulas which are A- or L-stable for arbitrary sizes k. The A-stable formulas are of order $k+2$ and the L-stable formulas are of order $k+1$ for $k\geqslant 2$.

The fatal defect of the implicit one-step block methods is inversion of large matrices during Newton-Raphson iterations. In this paper, we present a modified algorithm, which comes from a 4-block implicit method, and only two ordinary matrices need to be inversed for four new values.

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Some comparative numerical results are presented to show the efficiency of the modified algorithm.

§ 2. Block Implicit Methods with Nonequidistant Nodes

We shall be interested in obtaining a numerical solution of

$$y'(x)=f(x,y),\quad y(\alpha)=\eta,\quad \alpha\leqslant x\leqslant\beta, \tag{2.1}$$

where we make the usual assumptions that f is continuous and satisfies

$$|f(x,y)-f(x,z)|\leqslant L|y-z| \tag{2.2}$$

and on $[\alpha,\beta]\times(-\infty,\infty)$ the existence of a unique solution $y(x)\in C'[\alpha,\beta]$ is guaranteed. We shall assume that y has continuous derivatives on $[\alpha,\beta]$ of any order needed rather than make specific differentiability assumptions.

Now, let $x_{n+i}=x_n+\alpha_i h$, where $n=0, k, 2k, \cdots, 0<\alpha_i<k, i=1, \cdots, k-1, \alpha_k=k$ and $\alpha_i\neq\alpha_j$ when $i\neq j$. Define $a=(\alpha_1, \alpha_2, \cdots, \alpha_k)^T$ as a node vector. Let y_j denote the approximation of $y(x_j)$. The formulas we shall study may be put in the form

$$Y_{n,a}=y_n a^0+hBF(Y_{n,a})+hf_n b,\quad n=0, k, 2k, \cdots, \tag{2.3}$$

where $f_j=f(x_j, y_j)$, $a^0=(1, 1, \cdots, 1)^T$, $B=(b_{ij})_{k\times k}$, $b=(b_{10}, \cdots, b_{k0})^T$, $Y_{n,a}=(y_{n+1}, \cdots, y_{n+k})^T$, $F(Y_{n,a})=(f_{n+1}, \cdots, f_{n+k})^T$ and the initial value $y_0=\eta$. Equation (2.3) represents a system of non-linear equations for the new values which can be shown to have a unique solution if h is suitably small. In practice we may have to presume the existence of a solution.

With the block implict method (2.3) we associate a linear difference operator vector $\mathscr{L}$ defined by

$$\mathscr{L}[Y(x;a);h]=Y(x;a)-y_n a^0-hBY'(x;a)-hy'(x)b, \tag{2.4}$$

where $Y(x,a)=(y(x+\alpha_1 h), \cdots, y(x+\alpha_k h))^T$. Expanding the function $y(x+\alpha_j h)$ and its derivative $y'(x+\alpha_j h)$ as Taylor series about x and collecting terms in (2.4) give

$$\mathscr{L}[Y(x;a);h]=y(x)c_0+hy'(x)c_1+\cdots+h^q y^{(q)}(x)c_q+\cdots, \tag{2.5}$$

where c_q are constant vectors. A simple calculation yields the following formulas for the constant vectors c_q in terms of the coefficients a, B and b

$$\begin{cases} c_0=0, \\ c_1=a^1-Ba^0-b, \\ c_q=\dfrac{1}{q!}a^q-\dfrac{1}{(q-1)!}Ba^{q-1}, \quad q=2, 3, \cdots, n, \end{cases} \tag{2.6}$$

where $a^s=(\alpha_1^s, \cdots, \alpha_k^s)^T$.

For formula (2.3), we can state a convergence theorem.

Theorem 1. *Suppose we have a k-block implicit one-step method defined by (2.3), and let us assume the existence of v and $0<q\leqslant v$ such that the linear difference operator vector $\mathscr{L}$ satisfies $\|\mathscr{L}\|=O(h^{q+1})$ and $|(\mathscr{L})_k|=O(h^{v+1})$, where $(\mathscr{L})_k$ is the k-th component of $\mathscr{L}$. Then the method is convergent with global error of order h^p where $p=\min(v, q+1)$, that is $\|Y_{n,a}-Y(x;a)\|=O(h^p)$ for each $n=0, k, 2k, \cdots$, such that $x_{n+k}\leqslant\beta$, and the method is said to be of order p.*

The proof can be found in [10]. To obtain a higher order error, a few remarks seem noteworthy: First, we had better take q as large as possible. Second, advantage should be taken of formulas which are more accurate at the end of the block than in the interior.

From formulas (2.6), for a given node vector a, we can choose B and b as below (we restrict $n=k+1$),

$$\begin{cases} a^1-Ba^0-b=0, \\ a^q-qBa^{q-1}=0, \quad q=2, \cdots, k+1. \end{cases} \tag{2.7}$$

Let

$$A=(a^0, a^1, \cdots, a^{k-1}),$$
$$V=\text{diag}(\alpha_1, \cdots, \alpha_k), \quad (\text{we have } Va^q=a^{q+1}),$$
$$D_2=\text{diag}(2, 3, \cdots, k+1).$$

Obviously, A^{-1} and V^{-1} exist. Following (2.7), we have

$$\begin{cases} B=V^2AD_2^{-1}A^{-1}V^{-1}, \\ b=a^1-Ba^0. \end{cases} \tag{2.8}$$

If we define $a=(1, 2, \cdots, k)^T$, the B and b determined by (2.8) are then the same as those chosen by Shampine and Watts[10,11]. It can be proved that the associated block method converges in order $k+1$ for k odd and in order $k+2$ for k even, and that for $k=1, 2, \cdots, 8$ the method is A-stable and for $k=9$, 10 is not.

When formula (2.3) is applied to the usual scalar test equation $y'=\lambda y$, it is of the form

$$(I-\bar{h}B)Y_{n,a}=y_n(a^0+\bar{h}b),$$

where $\bar{h}=h\lambda$. Letting

$$x(\bar{h})=(I-\bar{h}B)^{-1}(a+\bar{h}b), \tag{2.9}$$

we have

$$Y_{n,a}=x(\bar{h})y_n. \tag{2.10}$$

In order to obtain the explicit expression of $x(\bar{h})$, we introduce the polynomial

$$\varphi(x)=(x-\alpha_1)(x-\alpha_2)\cdots(x-\alpha_k)=\sum_{i=0}^{k}(\varphi^{(i)}(0)/i!)\cdot x^i. \tag{2.11}$$

Lemma 1. *If B and b, the coefficients of the block method* (2.3), *are given by* (2.8), *we have*

$$x(\bar{h})=\sum_{i=0}^{k}p_i\bar{h}^i\Big/\sum_{i=0}^{k}r_i\bar{h}^i, \tag{2.12}$$

where

$$\begin{cases} r_i=(k-i+1)\cdot\varphi^{(k-i)}(0)/(k+1)! & (2.13a) \\ p_i=\sum_{s=0}^{i}r_{i-s}a^s/s! \quad i=0, 1, \cdots, k. & (2.13b) \end{cases}$$

Proof. From Cramer's rule, we can conclude that $x(\bar{h})$ has the form of (2.12). Multiplying by $\sum_{i=0}^{k}r_i\bar{h}^i\cdot(I-\bar{h}B)$ on both sides of (2.12) from left, we get

$$\sum_{i=0}^{k}p_i\bar{h}^i-B\sum_{i=0}^{k}p_i\bar{h}^{i+1}=\sum_{i=0}^{k}r_i\bar{h}^ia^0+\sum_{i=0}^{k}r_i\bar{h}^{i+1}b. \tag{2.14}$$

Equating corresponding coefficients in $\bar{h}^i$, we evidently obtain

$$\begin{cases} p_0 = r_0 a^0, & (2.15a)\\ p_i - Bp_{i-1} = r_i a^0 + r_{i-1} b, & (2.15b)\\ -Bp_k = r_k b, \quad i=1, \cdots, k. & (2.15c)\end{cases}$$

Without losing generality, we put $r_0=1$. Then we have $p_0=a^0$. This implies that (2.13b) is true for $i=0$. Suppose it is true for all indices through $i-1$, $i\leqslant k$. By (2.15b) and (2.7), we have

$$p_i = Bp_{i-1} + r_i a^0 + r_{i-1} b = B\sum_{s=0}^{i-1} r_{i-1-s} a^s/s! + r_i a^0 + r_{i-1} b$$

$$= \sum_{s=0}^{i-1} r_{i-1-s} a^{s+1}/(s+1)! + r_i a^0 + r_{i-1} a^1 = \sum_{s=0}^{i} r_{i-s} a^s/s!.$$

Thus (2.13b) holds for $i\leqslant k$. Substituting the p_k in (2.15c) by (2.13b), we have

$$-B\sum_{s=0}^{k} r_{k-s} a^s/s! = r_k(a^1 - Ba^0)$$

and from (2.7), we get

$$\sum_{s=0}^{k} r_{k-s} a^{s+1}/(s+1)! = 0. \tag{2.16}$$

Denote $u_s = (k+1)!\, r_{k-s}/(s+1)!$ and (2.16) becomes $\sum_{s=0}^{k} u_s a^s = 0$. That is, a_i, $i=1, \cdots, k$, are zeros of polynomial $\sum_{s=0}^{k} u_s x^s$. Since $u_k=1$, comparing with the polynomial $\varphi(x)$ defined by (2.11), we find

$$u_s = \varphi^{(s)}(0)/s!. \tag{2.17}$$

Hence

$$r_i = (k-i+1)\varphi^{(k-i)}(0)/(k+1)! \quad \blacksquare$$

Writing (2.10) in component forms, we have

$$y_{n+k} = \xi_k(\bar{h}) y_n = \xi_k^{\frac{n}{k}+1}(\bar{h}) y_0,$$

$$y_{n+i} = \xi_i(\bar{h}) y_n = \xi_i(\bar{h}) \xi_k^{\frac{n}{k}}(\bar{h}) y_0, \quad i=1, \cdots, k-1,$$

where $\xi_j(\bar{h})$ is the j-th component of the vector $x(\bar{h})$.

Definition. *The block implicit method (2.3) is said to be absolutely stable for a given $\bar{h}$ if, for that $\bar{h}$, $|\xi_k(\bar{h})|<1$. The region of absolute stability is defined as a set $S=\{\bar{h}\,|\,|\xi_k(\bar{h})|<1\}$. A block implicit method is said to be A-stable if $S\supset C^-$.*

§ 3. High Order A-stable Block Implicit One-step Methods

Once the node vector a is given, we can construct a block implicit method by (2.8). But the problem is how to choose a so as to optimize the block method, that is how to raise the order of the method as high as possible while keeping A-stability.

We quote a general definition: A rational approximation $R(z)$ to e^z is said to be A-acceptable, if $|R(z)|<1$ where Re $z<0$. It follows immediately that the A-stability of a one-step block method depends on the A-acceptability of the approximation $\xi_k(\bar{h})$ to $e^{k\bar{h}}$. It is known that if $R(z)$ is a diagonal Padé approximation to e^z, then $R(z)$ to e^z is A-acceptable (Birkhoff and Varga [2]).

The explicit expression of $[k/j]$ Padé approximation $\frac{P_k(z)}{Q_j(z)}$ to e^z is given below:

$$P_k(z)=\sum_{s=0}^{k}\frac{k!(j+k-s)!}{(k-s)!(j+k)!s!}z^s, \tag{3.1}$$

$$Q_j(z)=\sum_{s=0}^{j}(-1)^s\frac{j!(k+j-s)!}{(j-s)!(j+k)!s!}z^s. \tag{3.2}$$

Now, we introduce Jacobi's orthogonal polynomials on $[0, 1]$

$$\begin{aligned}P_n^{(\alpha,\beta)}(x)&=\frac{(-1)^n}{n!C_{2n+\alpha+\beta}^n(1-x)^\alpha x^\beta}\cdot\frac{d^n}{dx^n}[(1-x)^{n+\alpha}\cdot x^{n+\beta}]\\&=\sum_{s=0}^{n}\frac{C_{n+\alpha}^sC_{n+\beta}^{s+\beta}}{C_{2n+\alpha+\beta}^n}\cdot(x-1)^{n-s}\cdot x^s,\end{aligned} \tag{3.3}$$

where $P_n^{(\alpha,\beta)}(x)$ is a monic polynomial and associated with the weight function $\rho(x)=(1-x)^\alpha x^\beta$. The zeros of $P_n^{(\alpha,\beta)}(x)$ are real and distinct within the interval $[0, 1]$. Hence, it is possible for us to define $\varphi(x)$ as below:

$$\varphi(x)=x^kP_{k-1}^{(1,1)}(x/k)\cdot(x/k-1). \tag{3.4}$$

Lemma 2. *$\xi_k(\bar{h})$ is a diagonal Padé approximation to $e^{k\bar{h}}$ if the components of the node vector a are given by zeros of polynomial $P_{k-1}^{(1,1)}(x/k)(x-k)$ in magnitude order.*

Proof. First, we present two equalities about combinational numbers

$$\sum_{j=0}^{k}C_m^jC_n^{k-j}=C_{m+n}^k, \tag{3.5}$$

$$\sum_{t=0}^{u}(-1)^tC_u^t=\begin{cases}0, & u\neq0,\\1, & u=0.\end{cases} \tag{3.6}$$

(3.4), (3.3) imply

$$\begin{aligned}\varphi(x)&=k^kP_{k-1}^{(1,1)}(x/k)(x/k-1)=\sum_{s=0}^{k-1}\frac{C_k^sC_k^{s+1}}{C_{2k}^{k-1}}\sum_{j=0}^{k-s}(-1)^jk^jC_{k-s}^jx^{k-j}\\&=x^k+\sum_{j=1}^{k}(-1)^jk^j\Big(\sum_{s=0}^{k-j}\frac{C_k^sC_k^{s+1}}{C_{2k}^{k-1}}C_{k-s}^j\Big)x^{k-j}.\end{aligned}$$

Then, (2.13) and (3.5) yield

$$\begin{aligned}r_i&=(-1)^jk^j\frac{(k-j+1)!}{(k+1)!}\sum_{s=0}^{k-j}\frac{C_k^sC_k^{s+1}}{C_{2k}^{k-1}}\cdot C_{k-s}^j=(-1)^j\frac{k^jk!k!}{(2k)!j!}\sum_{s=0}^{k-j}C_{k-1}^s\cdot C_{k-j+1}^{k-j-s}\\&=(-1)^jk^j\frac{k!k!}{(2k)!j!}C_{2k-j}^{k-j}=(-1)^jk^j\frac{k!(2k-j)!}{(2k)!j!(k-j)!}.\end{aligned}$$

Comparing with (3.2), we get

$$\sum_{j=0}^{k}r_j\bar{h}^j=Q_k(k\bar{h}). \tag{3.7}$$

Then, (2.13b) implies

$$\begin{aligned}(p_j)_k&=\sum_{s=0}^{j}r_{j-s}k^s/s!=\sum_{s=0}^{j}(-1)^{j-s}k^j\frac{k!(2k-j+s)!}{(k-j+s)!(2k)!(j-s)!s!}\\&=k^j\frac{(2k-j)!}{(2k)!}\sum_{s=0}^{j}(-1)^sC_k^sC_{2k-s}^{j-s},\end{aligned}$$

Moreover, by (3.6) and (3.5), we have

$$
\begin{aligned}
(p_j)_k &= k^j \frac{(2k-j)!}{(2k)!} \sum_{t=0}^{j} (-1)^t C_k^t \sum_{s=0}^{j-t} C_{k-t}^{j-t-s} C_k^s \\
&= k^j \frac{(2k-j)!}{(2k)!} \sum_{s=0}^{j} C_k^s \sum_{t=0}^{j-s} (-1)^t C_k^t C_{k-t}^{j-t-s} \\
&= k^j \frac{(2k-j)!}{(2k)!} \sum_{s=0}^{j} C_k^s C_k^{j-s} \Big(\sum_{t=0}^{j-s} (-1)^t C_{j-s}^t \Big) \\
&= k^j \frac{(2k-j)!}{(2k)!} C_k^s = k^j \frac{(2k-j)!\,k!}{(2k)!\,j!\,(k-j)!}.
\end{aligned}
$$

Comparing with (3.1), we get

$$
\Big(\sum_{j=0}^{k} p_j \bar{h}^j \Big)_k = P_k(k\bar{h}). \tag{3.8}
$$

Combine (3.7) and (3.8) and the required result follows. ▮

Theorem 2. *The block implicit method* (2.3) *is A-stable if the node vector α is defined by Lemma* 2 *and B, b are given by* (2.8).

The remaining subject is the order of the methods. We first present the following lemma.

Lemma 3. *Assuming $P_k(x)$ is a polynomial which interpolates f at the nodes $\alpha_0=0$, α_1, $\cdots$, α_k, the components of the node vector, we have*

$$
\int_0^k f(x)dx = \int_0^k P_k(x)dx + R[f],
$$

where

$$
R[x^j]=0, \quad j=0,\ 1,\ \cdots,\ 2k-1.
$$

Proof. By the theory of interpolation, we have

$$
R[f] = \int_0^k f[x,\ \alpha_0,\ \cdots,\ \alpha_k]\cdot w_k(x)dx,
$$

where $f[x, \alpha_0, \cdots, \alpha_k]$ is the difference quotient and

$$
w_k(x) = x\cdot(x-\alpha_1)\cdots(x-\alpha_k) = x\cdot(x-k)\cdot k^{k-1} P_{k-1}^{(1,1)}(x/k).
$$

When $f(x)=x^j$, $j=0, 1, \cdots, 2k-1$, the difference quotient $f[x, \alpha_0, \cdots, \alpha_k]$ is a polynomial of degree $\leqslant k-2$. By the fact of orthogonality of $P_{k-1}^{(1,1)}(x/k)$, the result follows. ▮

Since the initial value problem $y'(x)=f(x, y(x))$, $y(x_n)=y_n$ is equivalent to the integral equation

$$
y(x) = y_n + \int_{x_n}^{x} f(t,\ y(t))dt,
$$

we approximate the integrals in

$$
y(x_{n+j}) = y_n + \int_{x_n}^{x_{n+j}} f(t,\ y(t))dt, \quad j=1,\ \cdots,\ k
$$

by integrating the k-th degree interpolating polynomial which agrees with $y'(x)$ at x_n, x_{n+1}, $\cdots$, x_{n+k}. Thus, we obtain a formula of the form (2.3) which is of order $k+1$. From (2.7), (2.8), we can conclude that the method of order $k+1$ is unique for a given node vector α. Hence, by Lemma 3, we obtain $|(\mathscr{L})_k| = O(h^{2k+1})$. That is $(c_{k+2})_k=0$ for $k\geqslant 2$. From Theorem 2, we obtain

Theorem 3. *The block implicit one-step method* (2.3) *is of order $k+2$ for $k\geqslant 2$*

and of order 2 for $k=1$ if the nodes are determined by Lemma 2 and the coefficients b and B are determined by (2.8). We denote them as ABIOS M's for short.

Jacobi's orthogonal polynomials $P_{k-1}^{(1,1)}(z/k)$ of $k\leqslant 4$ and their zeros are given below:

$$P_1^{(1,1)}(z/2)=\frac{1}{2}z-\frac{1}{2},\quad \alpha_1=1,$$

$$P_2^{(1,1)}(z/3)=\frac{1}{9}z^2-\frac{1}{3}z+\frac{1}{5},\quad \alpha_{1,2}=\frac{3}{2}\left(1\pm\sqrt{\frac{1}{5}}\right),$$

$$P_3^{(1,1)}(z/4)=\frac{1}{64}z^3-\frac{3}{32}z^2+\frac{9}{56}z-\frac{1}{14},\quad \alpha_{1,3}=2\left(1\pm\sqrt{\frac{3}{7}}\right),\ \alpha_2=2.$$

The coefficients b and B for $k\leqslant 4$ are displayed in Table 1.

Table 1 Coefficients of ABIOS M's for $k\leqslant 4$

$k=1$	$b=\begin{bmatrix}\frac{1}{2}\end{bmatrix}$	$B=\begin{bmatrix}\frac{1}{2}\end{bmatrix}$
$k=2$	$b=\begin{bmatrix}\frac{5}{12}\\ \frac{1}{3}\end{bmatrix}$,	$B=\begin{bmatrix}\frac{2}{3} & -\frac{1}{12}\\ \frac{4}{3} & \frac{1}{3}\end{bmatrix}$
$k=3$	$b=\begin{bmatrix}\frac{11}{40}+\frac{\sqrt{5}}{40}\\ \frac{11}{40}-\frac{\sqrt{5}}{40}\\ \frac{1}{4}\end{bmatrix}$	$B=\begin{bmatrix}(25-\sqrt{5})/40 & (25-13\sqrt{5})/40 & (-1+\sqrt{5})/40\\ (25+13\sqrt{5})/40 & (25+\sqrt{5})/40 & (-1-\sqrt{5})/40\\ 5/4 & 5/4 & 1/4\end{bmatrix}$
$k=4$	$b=\begin{bmatrix}\frac{17}{70}+\frac{3}{70}\sqrt{\frac{3}{7}}\\ \frac{13}{80}\\ \frac{17}{70}-\frac{3}{70}\sqrt{\frac{3}{7}}\\ \frac{1}{5}\end{bmatrix}$	$B=\begin{bmatrix}\frac{49}{90}-\frac{1}{10}\sqrt{\frac{3}{7}} & \frac{32}{45}-\frac{128}{105}\sqrt{\frac{3}{7}} & \frac{49}{90}-\frac{23}{30}\sqrt{\frac{3}{7}} & -\frac{3}{70}+\frac{3}{70}\sqrt{\frac{3}{7}}\\ \frac{49}{90}+\frac{49}{48}\sqrt{\frac{3}{7}} & \frac{32}{45} & \frac{49}{90}-\frac{49}{48}\sqrt{\frac{3}{7}} & \frac{3}{80}\\ \frac{49}{90}+\frac{23}{30}\sqrt{\frac{3}{7}} & \frac{32}{45}+\frac{128}{105}\sqrt{\frac{3}{7}} & \frac{49}{90}+\frac{1}{10}\sqrt{\frac{3}{7}} & -\frac{3}{70}-\frac{3}{70}\sqrt{\frac{3}{7}}\\ \frac{49}{45} & \frac{64}{45} & \frac{49}{45} & \frac{1}{5}\end{bmatrix}$

§ 4. High Order L-stable Block Implicit One-step Methods

The class of maximum order ($p=k+2$) methods have been found to be A-stable for arbitrary k. One drawback to these methods is their less than desirable asymptotic behavior. In particular, as $\lambda\to\infty$, $|\xi_k(h\lambda)|\to 1$, a point on the boundary rather than in the interior of the unit disk in the ξ-plane. In order to avoid this asymptotic behavior. Bichart and Picel[4] presented a subclass of implicit one-step methods of order $p=k$ with $b=0$; the nodes are equidistant yet. These methods are A-stable for $k=1$, 2 and stiffly stable for $k=3, \cdots, 25$. But if we make use of the advantage of nonequidistant nodes, we can easily construct a subclass of block implicit one-step methods, which are of order $p=k+1$ and L-stable for arbitrary k.

First, we put $b=0$ in (2.3), which leads to the form

$$Y_{n,a}=a^{*0}y_n+hB^*F(Y_{n,a}). \tag{4.1}$$

For a given node vector a^*, the largest value of q in Theorem 1, which can be reached, is k. That is, by (2.6), let

$$a^{*s}-sB^*a^{*s-1}=0, \quad s=1, 2, \cdots, k. \tag{4.2}$$

Making use of notations in Section 2 and assuming $D_1=\mathrm{diag}(1, 2, \cdots, k)$, we obtain

$$B^*=V^*A^*D_1^{-1}A^{*-1}. \tag{4.3}$$

When (4.1) is applied to the scalar test equation $y'=\lambda y$, it reduces to the form

$$Y_{n,a}=x^*(\bar{h})y_n,$$

where $\bar{h}=\lambda h$,

$$x^*(\bar{h})=(I-\bar{h}B^*)^{-1}a^0. \tag{4.4}$$

Definition. *The block implicit method* (2.3) *is said to be L-stable if it is A-stable and* $|\xi_k(\bar{h})|\to 0$ *as* $\mathrm{Re}\ \bar{h}\to-\infty$.

A rational approximation $R(z)$ to e^z is said to be L-acceptable if it is A-acceptable and satisfies $|R(z)|\to 0$ as $\mathrm{Re}\, z\to-\infty$. If $\xi_k^*(\bar{h})$ is a $[k-1/k]$ Padé approximation to $e^{k\bar{h}}$, $\xi_k^*(\bar{h})$ to $e^{k\bar{h}}$ is L-acceptable[5], and also the block method is L-stable.

The following lemmas and theorems are completely parallel to those in Sections 2 and 3. We only display them without proofs.

Lemma 4. *If* B^*, *the coefficient of block method* (4.1), *is given by* (4.3), *we have*

$$x^*(\bar{h})=\sum_{i=0}^{k-1}p_i^*\bar{h}^i\Big/\sum_{i=0}^{k}r_i^*\bar{h}^i, \tag{4.5}$$

where

$$r_i^*=\varphi^{*(k-i)}(0)/k!, \quad i=0, 1, \cdots, k,$$

$$p_i^*=\sum_{s=0}^{i}r_{i-s}^*a^{*s}/s!, \quad i=0, 1, \cdots, k-1.$$

where

$$\varphi^*(x)=(x-\alpha_1^*)\cdots(x-\alpha_k^*).$$

Lemma 5. $\xi_k^*(\bar{h})$ *is a* $[k-1/k]$ *Padé approximation to* $e^{k\bar{h}}$ *if the components of the node vector* a^* *are given by the zeros of polynomial* $P_{k-1}^{(1,0)}(x/k)(x-k)$ *in magnitude order.*

Theorem 4. *The block implicit method* (4.1) *is L-stable if the node vector* a^* *is defined by Lemma* 5 *and* B^* *is given by* (4.3).

Lemma 6. *Assuming* $P_k(x)$ *is a polynomial interpolating* f *at the nodes* $\alpha_1^*, \cdots, \alpha_k^*$, *the components of the node vector* a^*, *we have*

$$\int_0^k f(x)dx=\int_0^k P_k(x)dx+R[f],$$

where

$$R[x^j]=0, \quad \textit{for } j=0, 1, \cdots, 2k-2.$$

Theorem 5. *The block implicit one-step method* (4.1) *is of order* $k+1$ *for* $k\geq 2$ *and of order* 1 *for* $k=1$ *if the nodes are determined by Lemma* 5 *and the coefficients are determind by* (4.3). *We denote them as LBIOS M's for short.*

Jacobi's orthogonal polynomials $P_{k-1}^{(1,0)}(z/k)$ of $k\leq 4$ and their zeros are given below:

$$P_1^{(1,0)}(z/2)=\frac{1}{2}z-\frac{1}{3},\quad \alpha_1^*=\frac{2}{3},$$

$$P_2^{(1,0)}(z/3)=\frac{1}{9}z^2-\frac{4}{15}z+\frac{1}{10},\quad \alpha_{1,2}^*=\frac{3}{10}(4\pm\sqrt{6}),$$

$$P_3^{(1,0)}(z/4)=\frac{1}{64}z^3-\frac{9}{112}z^2+\frac{3}{28}z-\frac{1}{35},$$

$$\alpha_i^*=\frac{4}{7}\left(3+2\sqrt{2}\cos\left(\frac{\theta+2i\pi}{3}\right)\right),\quad i=1,\ 2,\ 3,$$

where $\theta=\cos^{-1}(\sqrt{2}/10)$. That is

$$\alpha_1^*=0.3543518378,\ \alpha_2^*=1.637867458,\ \alpha_3^*=3.150637847.$$

The coefficients B for $k\leqslant 4$ are displayed in Table 2.

Table 2 Coefficients of LBIOS M's for $k\leqslant 4$

$k=1$	$B^*=[1]$
$k=2$	$B^*=\begin{bmatrix}\frac{5}{6} & -\frac{1}{6}\\ \frac{3}{2} & \frac{1}{2}\end{bmatrix}$
$k=3$	$B^*=\begin{bmatrix}(88-7\sqrt{6})/120 & (296-169\sqrt{6})/600 & (-2+3\sqrt{6})/75\\ (296+169\sqrt{6})/600 & (88+7\sqrt{6})/120 & (-2-3\sqrt{6})/75\\ \frac{4}{3}-\frac{1}{12}\sqrt{6} & \frac{4}{3}+\frac{1}{12}\sqrt{6} & \frac{1}{3}\end{bmatrix}$
$k=4$	$B^*=\begin{bmatrix}0.4519979167 & -0.1612368826 & 0.1032095095 & -0.0396187060\\ 0.9375359826 & 0.8275702968 & -0.1914285128 & 0.0641896914\\ 0.8667271382 & 1.6244930562 & 0.7561460719 & -0.0967284193\\ 0.8818488444 & 1.5527738761 & 1.3153772792 & 0.2500000000\end{bmatrix}$

§ 5. Modified Algorithms

When we apply the block implicit method to a stiff system, the Newton-Raphson (N-R) iteration for solving the non-linear equation (2.3) or (4.1) is needed. During the N-R iteration, the matrix

$$DQ=I-hB\frac{\partial F(Y_{n,a})}{\partial Y_{n,a}}, \tag{5.1}$$

where

$$\frac{\partial F(Y_{n,a})}{\partial Y_{n,a}}=\operatorname{diag}(J_{n+1},\ \cdots,\ J_{n+k})$$

if we denote

$$J_v=\left(\frac{\partial f}{\partial y}\right)(x_v,\ y_v)$$

needs inversing. If (2.1) is a system containing m differential equations, DQ is a $km\times km$ square matrix far larger than what is to be inversed in other implicit linear methods. The algorithm will require much work on them. It may be the fatal defect of the block implicit methods. In this section, we shall modify the iteration, so that only matrices of order m need to be inversed. We only discuss the case $k=4$. For the convenience, we assume that $m=1$, which is easy to be generalized to any m. When $m=1$, J_v is a real number.

Since $y_{n+1}, \cdots, y_{n+4}$ are unknown before iteration, we should use other approaches to approximate the matrix $\frac{\partial F(Y_{n,a})}{\partial Y_{n,a}}$. For example, we may use

$$\frac{\partial F}{\partial Y}=J_{n+u}I_4, \quad 0\leqslant u\leqslant 4 \tag{5.2}$$

to approximate it, and hold it constant throughout the N-R iterations.

Since B, when $k=4$, have two pairs of conjugate complex eigenvalues $\lambda_1, \bar{\lambda}_1=u_1\pm v_1 i$, $\lambda_2, \bar{\lambda}_2=u_2\pm v_2 i$ and corresponding eigenvectors $\xi_1\pm\eta_1 i$, $\xi_2\pm\eta_2 i$. We have a factorization

$$B=XAX^{-1}, \tag{5.3}$$

where

$$A=\begin{bmatrix} A_1 & 0 \\ 0 & A_2 \end{bmatrix} \tag{5.4}$$

if we let

$$A_i=\begin{bmatrix} u_i & v_i \\ -v_i & u_i \end{bmatrix}, \quad i=1, 2;$$

and

$$X=(\xi_1, \eta_1, \xi_2, \eta_2). \tag{5.5}$$

Moreover, by denoting $\bar{Y}_{n,a}=X^{-1}Y_{n,a}$; $\bar{a}=X^{-1}a$; $\bar{b}=X^{-1}b$; $\bar{B}=AX^{-1}$ and $\bar{F}(\bar{Y}_{n,a})=F(X\bar{Y}_{n,a})=F(Y_{n,a})$, (2.3) then turns out to be of the form

$$\bar{Y}_{n,a}=y_n\bar{a}^0+h\bar{B}\bar{F}(\bar{Y}_{n,a})+hf_n\bar{b}, \tag{5.6}$$

the non-linear equation for $\bar{Y}_{n,a}$. To solve this equation, we still use N-R iterations, that is

$$\bar{Y}^{(s+1)}_{n,a}=\bar{Y}^{(s)}_{n,a}-D\bar{Q}(\bar{Y}^{(s)}_{n,a})^{-1}\bar{Q}(\bar{Y}^{(s)}_{n,a}), \tag{5.7}$$

where

$$\bar{Q}(\bar{Y}^{(s)}_{n,a})=\bar{Y}^{(s)}_{n,a}-y_n\bar{a}^0-h\bar{B}\bar{F}(\bar{Y}_{n,a})-hf_n\bar{b},$$

$$D\bar{Q}(\bar{Y}^{(s)}_{n,a})=I-h\bar{B}\frac{\partial\bar{F}(\bar{Y}_{n,a})}{\partial\bar{Y}_{n,a}}. \tag{5.8}$$

By the definition of the partial derivative and the facts that $\bar{F}(\bar{Y}_{n,a})=F(Y_{n,a})$, $\bar{Y}_{n,a}=x^{-1}Y_{n,a}$, we can conclude

$$\frac{\partial\bar{F}(\bar{Y}_{n,a})}{\partial\bar{Y}_{n,a}}=\frac{\partial F(Y_{n,a})}{\partial Y_{n,a}}X.$$

Replacing it into (5.8), we obtain

$$D\bar{Q}(\bar{Y}^{(s)}_{n,a})=I-h\bar{B}\frac{\partial F(Y_{n,a})}{\partial Y_{n,a}}X.$$

Using the approximation (5.2) and the fact that $\frac{\partial F}{\partial Y}$ and X are exchangeable yields

$$D\bar{Q}(\bar{Y}^{(s)}_{n,a})\cong D\bar{Q}=I_4-hJ_{n+v}A. \tag{5.9}$$

Obviously, the matrix $D\bar{Q}$ has a special form

$$D\bar{Q}=\begin{bmatrix} I-hJ_{n+v}A_1 & 0 \\ 0 & I-hJ_{n+v}A_2 \end{bmatrix} \tag{5.10}$$

and the iteration (5.6) turns out to be of the form

$$\overline{Y}^{(s+1)}_{n,a} = \overline{Y}^{(s)}_{n,a} - D\overline{Q}^{-1}\cdot\overline{Q}(\overline{Y}^{(s)}_{n,a}). \tag{5.6$'$}$$

Thus, the inversion of matrix DQ reduces to the inversion of matrices $I-hJ_{n+v}\Lambda_i$, $i=1, 2$. A simple calculation yields

$$(I_2-hJ_{n+v}\Lambda_i)^{-1}=\{1-2u_ihJ_{n+v}+|\lambda_i|^2h^2J^2_{n+v}\}^{-1} \times\{I_2-hJ_{n+v}\Lambda_i^T\},\quad i=1,\ 2 \tag{5.11}$$

Obviously, all formulas are true for a differential system, if we consider $\frac{\partial f}{\partial y}$ as a matrix of order m. In this way, for size $k=4$, only two matrices of order m need to be inversed for four new values. The amount of work in N–R iterations of block implicit methods is considerably reduced. The coefficients of the modified algorithm by ABIOS, denoted as ABIOS–4, are given in Table 3.

Table 3 Coefficients of ABIOS–4

$$X=\begin{bmatrix} 0.1633653035 & 0.0511856316 & 0.0103142837 & 0.0330880422\\ 0.4097513700 & -0.3963268524 & -0.1167772031 & -0.0972023015\\ 1.5512217231 & -3.5910231211 & 0.4417439054 & -0.2782421936\\ 1.0000000000 & -10.6238099656 & 1.0000000000 & 0.3456022647 \end{bmatrix}$$

$$\overline{B}=\Lambda X^{-1}=\begin{bmatrix} 2.412540972 & 0.213336136 & 0.137150656 & -0.0605563010\\ -0.195330074 & -0.381461600 & 0.0369379598 & -0.0588484475\\ -4.919509188 & -1.989866519 & 1.292853712 & -0.386475119\\ 4.400166517 & -2.470536311 & 0.148455004 & 0.0631844729 \end{bmatrix}$$

$$\overline{a}^0=X^{-1}a^0=\begin{bmatrix} 4.17307072914\\ 0.30485398027\\ -3.46939650631\\ 10.22862663890 \end{bmatrix}\qquad \overline{b}=X^{-1}b=\begin{bmatrix} 1.07328023096\\ 0,13401421513\\ -0.42160582418\\ 2.81267586997 \end{bmatrix}\qquad \begin{aligned} u_1&=0.6337350381\\ v_1&=0.1897640521\\ u_2&=0.3662649619\\ v_2&=-0.4626504521 \end{aligned}$$

Standard Scheme. Let the previously computed values y_n, f_n be preserved.

Stage 1. Let $\overline{Y}_{n,a}:=y_n\overline{a}^0$; $x_{n+i}:=x_n+\alpha_ih$; $i=1, \cdots, 4$; $F_{n+k}=F(Y_{n,a}):=f_na^0$.

Stage 2. If $\|hf_n\|_\infty\leqslant 0.05$, then $y_{n+v}:=y_n$. Else let y_{n+v} be the value at x_{n+2} of Lagrange interpolation at the values y_{n-2}, y_{n-1}, y_n. Then, evaluate the Jacobian matrices $\frac{\partial f}{\partial y}$ and $\left(\frac{\partial f}{\partial y}\right)^2$ at the value y_{n+v}.

Stage 3. Let

$$T_i:=I-2u_ih\left(\frac{\partial f}{\partial y}\right)_{n+v}+|\lambda_i|^2h^2\left(\frac{\partial f}{\partial y}\right)^2_{n+v},\quad i=1,\ 2,$$

and compute the L_iU_i factors of the resulting T_i, $i=1, 2$.

Stage 4. Let

$$\overline{Q}(\overline{Y}^{(s)}_{n,a})=(\overline{q}_1, \cdots, \overline{q}_4):=\overline{Y}^{(s)}_{n,a}-y_n\overline{a}^0-h\overline{B}F_{n+k}-hf_n\overline{b}$$

and then compute

$$\begin{bmatrix} q_1\\ q_2 \end{bmatrix}:=S_1\begin{bmatrix} \overline{q}_1\\ \overline{q}_2 \end{bmatrix},\quad \begin{bmatrix} q_3\\ q_4 \end{bmatrix}:=S_2\begin{bmatrix} \overline{q}_3\\ \overline{q}_4 \end{bmatrix},$$

where

$$S_i=I-h\cdot\left(\frac{\partial f}{\partial y}\right)_{n+v}\cdot\Lambda_i^T,\quad i=1,\ 2.$$

Stage 5. Solve the equations

$$\begin{cases} T_1\delta_i^{(s)}=L_1U_1\delta_i^{(s)}=q_i, \\ T_2\delta_{i+2}^{(s)}=L_2U_2\delta_{i+2}=q_{i+2}, \quad i=1,\ 2, \end{cases}$$

and let

$$\overline{Y}_{n,a}^{(s+1)}=\overline{Y}_{n,a}^{(s)}-\delta^{(s)},$$

where

$$\delta^{(s)}=(\delta_1^{(s)},\ \cdots,\ \delta_4^{(s)}).$$

Stage 6. Allow $\leqslant 4$ N-R iterations and, if they converge, let $Y_{n,a}=X\overline{Y}_{n,a}$ and $f_{n+k}=f(x_{n+k},\ y_{n+k})$, which can be accepted. Proceed to Stage 7. Otherwise, let $F_{n,a}=F(X\overline{Y}_{n,a}^{(s+1)})$ and add 1 to index s; return to Stage 4.

Stage 7. Estimate the new step size h for next step and update $x_n:=x_{n+k}$, $y_n:=y_{n+k}$, $f_n:=f_{n+k}$; return to Stage 1.

Given a standard LU factorization routine, the above scheme is not difficult to program.

§ 6. Numerical Results

Example 1. Krogh has proposed the following example to test programs for stiff equations ([7], pp. 218—219):

$$y'(x)=-By(x)+U(z_1^2,\ z_2^2,\ z_3^2,\ z_4^2),\ y_i(0)=-1,\ i=1,\ \cdots,\ 4;\ x\in[0,\ 1000], \tag{6.1}$$

where

$$\begin{cases} U=\dfrac{1}{2}\begin{bmatrix} -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \end{bmatrix},\quad U^{-1}=U, \\ B=U\cdot\mathrm{diag}(\beta_1,\ \beta_2,\ \beta_3,\ \beta_4)\cdot U, \\ z=U\cdot y. \end{cases} \tag{6.2}$$

Obviously, if we take transformation $z=Uy$, (6.1) reduces to the form

$$z_i'=-\beta_i z_i+z_i^2,\quad z_i(0)=-1,\quad i=1,\ \cdots,\ 4.$$

The solution is

$$z_i=\frac{\beta_i}{1+c_ie^{\beta_ix}},\quad i=1,\ \cdots,\ 4,$$

where

$$c_i=-(1+\beta_i).$$

In the light of Krogh's suggestion, the problem is integrated with $\beta_1=1000$, $\beta_2=800$, $\beta_3=-10$ and $\beta_4=0.001$. Initially, the eigenvalues are -1002, -802, -8 and -2.001. When $0.001x\gg1$, they are -1000, -800, -10 and -0.001.

The initial step-size $h_0=10^{-4}$ and then the tolerance $\varepsilon=10^{-5}$. The numerical results by ABIOS-4 compared with Gear's published results[7] at the first step to pass 10^i for $i=-2,\ -1,\ \cdots,\ 3$ are given in Table 4.

Table 4 Integration of Krogh Problem by ABIOS-4 and GEAR

ABIOS-4/GEAR					
Present error	Steps	Evaluations	LU/Inv.	Average step	Current time
.185D-6/.910D-7	6×4/70	35/179	12/7	4.34D-4/1.463D-4	.0104149/.01024367
.656D-5/.267D-5	10×4/110	71/262	20/12	3.09D-3/9.535D-4	.114166/.1048869
.77D-7/.221D-5	16×4/168	141/405	32/15	1.57D-2/6.025D-3	1.00201/1.0122667
.112D-5/.287D-5	22×4/216	195/523	44/20	1.20D-1/4.635D-2	10.4868/10.0110786
.861D-6/.298D-5	26×4/252	231/616	52/25	9.34D-1/4.067D-1	101.276/102.477128
.345D-5/.120D-5	30×4/283	263/693	60/29	8.33D00/3.625D00	1000.00/1025.77693

Example 2. Problem B_5 from Enright[6], with eigenvalues close to imaginary axis.

$$\begin{cases} y_1' = -10y_1 + \alpha y_2, & y_1(0) = 1, \\ y_2' = -\alpha y_1 - 10y_2, & y_2(0) = 1, \\ y_3' = -4y_3, & y_3(0) = 1, \\ y_4' = -y_4, & y_4(0) = 1, \\ y_5' = -0.5y_5, & y_5(0) = 1, \\ y_6' = -0.1y_6, & y_6(0) = 1; \end{cases}$$

terminal value $x_f = 20$, $h_0 = 10^{-3}$; $\alpha = 100$.

The eigenvalues are: -0.1, -0.5, -1, -4, $-10 \pm 100i$; the tolerance $\varepsilon = 10^{-4}$.

Integration of problem B_5 is extremely difficult by Gear's method. But ABIOS-4 has the advantage. The numerical results compared with those by GEAR, SDBASIC, TRAPPEX, GENRK, IMPRK are given in Table 5, where NJ is the number of Jacobian evaluations required to solve the problem and ERR OVER the maximum global error over all steps in the solution of the problem.

Table 5 Integration of Problem B_5

Methods	Evaluations	NJ	LU	Steps	Max error	ERR OVER
ABIOS-4	261	52	104	208	1.3E-4	0.019
GEAR	6738	24	24	2752	1.0E-4	0.003
SDBASIC	352	352	17	117	0.6E-4	0.0
TRAPEX	1265	17	17	178	0.8E-4	0.0
GENRK	867	20	60	77	2.3E-4	0.039
IMPRK	1057	13	13	83	0.7E-4	0.0

A large number of stiff problems have been successfully solved using the above scheme. ABIOS-4 was implemented in Fortran, and was run on a microcomputer. The scheme can yield better results if run on a larger-capacity computer.

§ 7. Conclusion

A class of A-stabe and L-stable block implicit one-step methods with nonequidistant nodes have been described and used for the integration of stiff systems of O.D.E.s. The order of A- and L-stable methods can be arbitrarily high. The amount of work of the modified algorithm is considerablely reduced in iteration, which makes the block methods useful. The scheme in Section 5 is easy to implement. The method compares favourably with Gear's method. Also, for some problems with eigenvalues close to the imaginary axis, the ABIOS-4 can be much more efficient than Gear's method. This may be of importance in some areas, for example, for problems arising in circuit analysis. Finally we note that there is much work yet to be done in implementing block methods in an efficient manner. In particular it is clear that the problems of reducing the number of LU decompositions and of effectively controlling the global error need further investigation.

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