A New Block Method and Their Application to Numerical Solution of Ordinary Differential Equations

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Abstract: A class of multistage and multistep integration methods which can obtain \( r \) new values simultaneously at each integration step was developed. Their stability regions were derived and sketched by MATLAB, and their regions are either A-stable or \( A(\alpha) \)-stable. Their applications to numerical solutions of nonstiff and stiff equations by predictor-corrector scheme were also studied.

1. Introduction

Numerical solutions for ordinary differential equations (ODEs) have great importance in scientific computation, as they were widely used to model in representing the real world problems. The common methods used to solve ODEs are categorized as one-step (multistage) methods and multistep (one stage) methods, which Runge-Kutta methods represent the former group, and Adams-Bashforth-Molton method represents the later group [5]. Some multistage methods are also available in the community. Implicit one-step method has been studied by Stoller and Morrison [9], Butcher [2], Fang [4], and Shampine and Watts [10]. We will consider a class of explicit and implicit with multistep and multistage methods for solving ordinary differential equations; we can call it a block method [1,6,7]. This method can obtain a block of new values simultaneously which makes its computation be competitive, and especially its implicit type formulas can be used in solving stiff ODEs effectively. Our aim of this paper is to sketch their stability regions to know how they can be implemented effectively in numerical implementation. The size of stability region of a numerical method is especially important in the choice of methods suitable for solving stiff system. Indeed, for numerical solution of stiff systems, it requires an interval of stability region to be as large as possible to avoid restricted stepsize implementation during numerical integration. A method with large interval of stability may be sufficient in the integration for stiff ODEs; for example, when the Jacobian matrix of right-hand side function has eigenvalues which are located in a large, narrow strip along the negative real axis. Such equations often arise when a second order hyperbolic differential equations in semi-discretized with respect to space variable [11].
This paper is organized as follows. In section 2, we will show some block multistage/multistep method, and their stability regions will be sketched and be given in section 3. In section 4, a fixed stepsize and a variable stepsize implementation for numerical solutions of nonstiff and mildly stiff ODEs by Block formulas are implemented. Their numerical results show its efficiency and effectiveness. Section 5 gives the conclusion.

2. Block Multistage and Multistep Method

Given a class of s stages and m steps integration formulas [1,6,7], where
\[ h^{-1}(\sum_{j=0}^{m} k_j y_{i+q-1}) \] approximates \( y'(x_{i+q}) \) of order \( h^m \), \( q = 1, 2, \ldots, s \). Derivation is skipped here and a few formulas are given in the following:

a. For \( s=m=1 \), it is exactly the same as the classical BDF formula.

b. For \( s=2, m=3 \), explicit and implicit formula are the following:

\[
\begin{align*}
2y_{i+2} - 9y_{i+1} + 18y_i - 11y_{i-1} &= 6hf(x_{i-1}, y_{i-1}) \\
y_{i+2} + 6y_{i+1} - 3y_i - 2y_{i-1} &= 6hf(x_i, y_i)
\end{align*}
\] (2.1)

\[
\begin{align*}
2y_{i+2} + 3y_{i+1} - 6y_i + y_{i-1} &= 6hf(x_{i+1}, y_{i+1}) \\
11y_{i+2} - 18y_{i+1} + 9y_i - 2y_{i-1} &= 6hf(x_{i+2}, y_{i+2})
\end{align*}
\] (2.2)

c. For \( s=2, m=4 \), an implicit formula is the following:

\[
\begin{align*}
3y_{i+2} + 10y_{i+1} - 18y_i + 6y_{i-1} - y_{i-2} &= 12hf(x_{i+1}, y_{i+1}) \\
25y_{i+2} - 48y_{i+1} + 36y_i - 16y_{i-1} + 3y_{i-2} &= 12hf(x_{i+2}, y_{i+2})
\end{align*}
\] (2.3)

d. For \( s=3, m=5 \), explicit and implicit formulas are the following:

\[
\begin{align*}
-12y_{i+3} - 75y_{i+2} + 200y_{i+1} - 300y_i + 300y_{i-1} - 137y_{i-2} &= 60hf(x_{i-2}, y_{i-2}) \\
-3y_{i+3} + 20y_{i+2} - 60y_{i+1} + 120y_i - 65y_{i-1} - 12y_{i-2} &= 60hf(x_{i-1}, y_{i-1}) \\
2y_{i+3} - 15y_{i+2} + 60y_{i+1} - 20y_i - 30y_{i-1} + 3y_{i-2} &= 60hf(x_i, y_i)
\end{align*}
\] (2.4)

\[
\begin{align*}
-3y_{i+3} + 30y_{i+2} + 20y_{i+1} - 60y_i + 15y_{i-1} - 2y_{i-2} &= 60hf(x_{i+1}, y_{i+1}) \\
12y_{i+3} + 65y_{i+2} - 120y_{i+1} + 60y_i - 20y_{i-1} + 3y_{i-2} &= 60hf(x_{i+2}, y_{i+2}) \\
137y_{i+3} - 300y_{i+2} + 300y_{i+1} - 200y_i + 75y_{i-1} - 12y_{i-2} &= 60hf(x_{i+3}, y_{i+3})
\end{align*}
\] (2.5)
These formulas can be implemented by either Newton iteration with respect to implicit formulas or by predictor-corrector schemes. In this paper, we only implement by a predictor-corrector scheme to see how its implementation in nonstiff and mildly stiff ODEs. Implicit solutions of this block method will be given elsewhere. The block PECE numerical results are given at section 4.

2. Stability regions

The main difficulty associated with stiff equations is that even though the component of the true solutions corresponding to some eigenvalues that may becoming negligible, the restriction on the stepsize imposed by the numerical stability of the method requires that $|h\lambda|$ remain small throughout the range of integration. So a suitable formula for stiff equations would be the one that would not require that $|h\lambda|$ remains small. Dahlquist [3] investigated the special stability problem connected with stiff equations, he introduced the concept of A-stability, and we quote the definition as the following:

**Definition 3.1 [3,5]:** The stability region $R$ associated with a multistep formula is defined as the set

$$R = \{ h\lambda : \text{A numerical formula applied to } y' = \lambda y, \, y(x_0) = y_0, \text{ with constant stepsize } h > 0, \text{ produce a sequence } (y_n) \text{satisfying that } y_n \to 0 \text{ as } n \to \infty \}.$$

**Definition 3.2 [3,5]:** A formula is A-stable if the stability region associated with that formula contains the open left half complex place.

**Definition 3.3 [3,5]:** A convergent linear multistep method is $A(\alpha)$-stable, $0 < \alpha < \pi / 2$, if

$$S \supset S_\alpha = \{ \mu : |\arg(-\mu)| < \alpha, \, \mu \neq 0 \}.$$ A method is A(0)-stable if it is $A(\alpha)$-stable for some (sufficiently small) $\alpha > 0$. To derive the absolute stability, one may consider the model problem (2). We apply formulas Eqs. 2.1~2.2, and 2.5 to $y' = \lambda y, \, y(x_0) = y_0$, and manipulation is skipped.

Let $\mu = \lambda h$, we have the following results:

**a.** Formula 2.1, 2.2 respectively.
We notice that at Figure 3.3, the stability region shows that Formula 2.5 is an $A(\alpha)$-stable method, which means the region covers almost all the left half plan. It is crucial to implement in stiff differential equation.

In this paper, we are trying to use a cheap implementation method to solve some mildly stiff ODEs, which is a standard PECE scheme. Though an implicit implementation is also possible, but
in consideration of the high cost of Jacobian evaluations, we would like to know how good this cheap scheme with block formulas can lead us to. For the stability region of the numerical Predictor-Corrector scheme, we can approach by the following. Let $H = h\lambda$. We could rewrite Eqs. 2.1 and 2.2 by the following, Eqs. 2.4 and 2.5 is done by exactly the same way, we do not give the details here.

\[
Y^p_m = AY^c_{m-1} + hBF^c_{m-1}
\]

\[
Y^c_m = A^*Y^c_{m-1} + hB^*F^p_m
\]

where

\[
\begin{bmatrix}
y^p_{n+1} \\
y^p_{n+2}
\end{bmatrix} = \begin{bmatrix}
5 & -4 \\
28 & -27
\end{bmatrix} \begin{bmatrix}
y^c_{n-1} \\
y^c_n
\end{bmatrix} + 6h \begin{bmatrix}
\frac{1}{3} & \frac{2}{3} \\
2 & 3
\end{bmatrix} \begin{bmatrix}
f^c_{n-1} \\
f^c_n
\end{bmatrix}
\]

(3.2)

and

\[
\begin{bmatrix}
y^c_{n+1} \\
y^c_{n+2}
\end{bmatrix} = \begin{bmatrix}
-5 & 28 \\
23 & 23
\end{bmatrix} \begin{bmatrix}
y^c_{n-1} \\
y^c_n
\end{bmatrix} + 6h \begin{bmatrix}
11 & -2 \\
69 & 69
\end{bmatrix} \begin{bmatrix}
f^c_{n-1} \\
f^c_{n+2}
\end{bmatrix}
\]

(3.3)

or in matrix formulation

\[
Y^p_m = AY^c_{m-1} + HB^c
\]

(3.4)

and

\[
Y^c_m = A^*Y^c_{m-1} + HB^* \left( AY^c_{m-1} + HB^c \right)
\]

\[
= \left( A^* + HB^* + H^2 B^* B \right) Y^c_{m-1}
\]

(3.5)

Define

\[
P(H) = \left( A^* + HB^* + H^2 B^* B \right)
\]

(3.6)

Then the locus of H determines the boundary of the stability region and can be plotted by MATLAB as the following. We use one predictor and one corrector and denote it as $PE(CE)^1$. More iteration of correctors can be derived similarly.
The region is the interior of the blue line

Without further derivation, we also present a stability region by using $s=2$, $m=3$, which is Eq. 2.1 as a predictor, and $s=2$, $m=4$, which is Eq. 2.3 as a corrector. We derive a similar locus plot as the following:

The region is the interior of the blue line

Define $H^* = \sup \{ - H | \rho(P(H)) < 1, H = \lambda h, \text{Re}(\lambda) < 0 \}$. From Figures 3.4 and 3.5, the largest intercept is about -2.5. According to [4,8,10], their interval of intercept are all less than 1. That makes our scheme has a better control of the length of stepsize in the integration when it is implemented by variable stepsize strategy.

3. Numerical Experiments

We will show few examples to see the results of applying a variable stepsize selection strategy, which readers may refer to [3] and a block Predictor-Corrector numerical scheme on both nonstiff and mildly stiff ODEs. The effectiveness of obtaining many step-points value in each iteration drive us to derive new block formulas to take advantage of this efficiency of our new method. It can help
us in the future to solve many application problems, such as simulation of multibody problems, and flexible mechanism.

**Example 1:** A nonstiff ODE. \( y' = -\lambda y, \quad y(0) = 1, \quad t \in [0,5]. \)
The exact solution is \( y = e^{-\lambda t}. \) Case 1: \( \lambda = 1. \)

![Figure 4.1: Block PECE numerical solution with \( \lambda = 1 \)](image)

![Figure 4.2: Absolute error log plot with fixed stepsize when \( \lambda = 1 \) (the y-axis is \( 10^{-11} \sim 10^{-13.5} \))](image)

![Figure 4.3: Absolute error log plot with variable stepsize when \( \lambda = 1 \) (the y-axis is \( 10^{-9.8} \sim 10^{-10.5} \))](image)

**Example 2:** A mild stiff ODE. \( y' = -\lambda y, \quad y(0) = 1, \quad t \in [0,5]. \)
The exact solution is \( y = e^{-\lambda t}. \) Case 2: \( \lambda = 60 \)
Figure 4.4: Block PECE numerical solution with $\lambda = 60$

Figure 4.5: Absolute error log plot with variable stepsize when $\lambda = 60$

(the size of y-axis is $10^{-5} \sim 10^{-12}$)

Example 3:

\[ y'_1 = -y_2 - y_1 y_3 / r \]
\[ y'_2 = y_1 - y_2 y_3 / r \]
\[ y'_3 = y_1 / r \]

, where \[ r = \sqrt{y_1^2 + y_2^2} \], \[ y_1(0) = 3 \]
\[ y_2(0) = 0 \], \[ t \in [0, 20] \]
\[ y_3(0) = 0 \]

True solutions:

\[ y_1 = (2 + \cos(t)) \cos(t) \]
\[ y_2 = (2 + \cos(t)) \sin(t) \]
\[ y_3 = \sin(t) \]

Figure 4.6: Block PECE numerical solutions
In example 1, it is a nonstiff ODE. Figure 4.1 gives the trace of the numerical solution, Figure 4.2 gives the accuracy of the numerical solution when \( h = 10^{-3} \) by fixed stepsize implementation. The accuracy is about \( 10^{-11} \). In Figure 4.3, the accuracy is about \( 10^{-10} \) by variable stepsize implementation. In example 2, it is a mildly stiff ODE. Figure 4.5 gives the accuracy, and it is about \( 10^{-9} \) by variable stepsize implementation. In Example 3, it is a mildly stiff ODEs with three components. The accuracy is almost the same in example 2 which is about \( 10^{-9} \sim 10^{-10} \) in three components. As in [7], we have shown that this block method is of order 3 when \( s=2, m=3 \). For these figures, we know the method is accurate, especially in nonstiff ODEs.

### 4. Conclusion

In this paper, we have derived several new block numerical schemes with different stages \( s \) and steps \( m \). Absolute stability regions of several methods have been sketched and a predictor corrector scheme by these block formula is established, their intercept of stability region is the best among known results in articles. In addition, numerical results by implementing predictor corrector scheme
to some nonstiff and mildly stiff ODEs are obtained, the numerical results show the method is
effective and accurate regarding to be able to obtain many step-points values in each iteration and
rate of convergence respectively.

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