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A Short Communication

NEW HIGH-ORDER IMPLICIT RUNGE-KUTTA METHODS AND APPLICATIONS TO PARALLEL INTEGRATIONS[1]

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1. INTRODUCTION

An s-stage implicit Runge-Kutta method (IRK method) for numerically solving the initial value problem (IVP) $\boldsymbol{y}'(t) = \boldsymbol{f}(\boldsymbol{y}(t))$, $\boldsymbol{y}(0) = \boldsymbol{y}_0$ is specified by the Butcher array

$$\begin{array}{c|c} \mathbf{c} & A \\ \hline & \boldsymbol{b}^T \end{array}$$

where $\boldsymbol{c}$, $\boldsymbol{b}$ are s-dimensional vectors, and A is a s-by-s matrix. For an s-stage collocation IRK method based on the collocation vector $\boldsymbol{c} = (c_1, \ldots, c_s)^T$ with distinct abscissas c_j, the parameter vector of weights $\boldsymbol{b} = (b_1, \ldots, b_s)^T$ and RK matrix $A = (a_{ij})$, $i, j = 1, \ldots, s$, are defined by the simplifying conditions $B(s)$ and $C(s)$ (cf. e.g., [6], [9]).

In the literature a number of classes of high- order A-stable implicit Runge-Kutta methods was proposed: Gauss-Legendre, Radau IA, IIA and Lobatto IIIA, IIIB, IIIC (cf. [1], [2], [4], [5], [7] [14]). A-stability of these high-order IRK methods was obtained by applying A-stability of the associated Padé approximation to the exponential function.

The above mentioned IRK methods belong nowadays to the set of the best methods of this type. However, in actual large-scale scientific computation when a parallel algorithm based on these IRK methods (cf. e.g., [11], [12], [13]) has to be designed, the freedom on the choice

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of the method parameters has the advantage of improving the efficiency of the related parallel algorithms. As for an example of this situation we mention the research reported in [15] where the freedom on the choice of the parameters of symmetric RK methods were used to improve the rate of convergence of the parallel iteration process. In this paper in order to have some degrees of freedoms we consider the s-stage collocation IRK methods based on s-dimensional *extended* Gauss collocation vector. This s-dimensional extended Gauss collocation vector is obtained by adding one component denoted by c to the original $(s-1)$-dimensional Gauss collocation vector. This additional component c assumes to be a free parameter. As the result we obtain an s-stage IRK method depending on the free additional abscissa c of the collocation vector. This method will be denoted by RK (s, c). By this way we sacrify the nice property of superconvergence of the Butcher's methods. However, it can be shown (cf. Subsection 2.1) that the new s-stage RK (s, c) is still of order $2s-2$. Moreover they are strongly A-stable for $c > 1/2$ and L-stable for $c = 1$ (cf. Subsection 2.2). Table 1.1 summarizes the main characteristics of the high-order IRK methods available in the literature and of the one-parameter family of new RK (s, c) methods considered in this paper.

Table 1.1. Summary of main characteristics of s-stage IRK methods

IRK methods	Order	Stage order	Stability properties	Original references
Gauss-Legendre	$2s$	s	A-stable for all s	Butcher [2]
Radau IA	$2s-1$	$s-1$	L-stable for all s	Ehle [7]
Radau IIA	$2s-1$	s	L-table for all s	Ehle [7], Axelsson [1]
Lobatto IIIA	$2s-2$	s	A-stable for all s	Ehle [7]
Lobatto IIIB	$2s-2$	$s-2$	A-stable for all s	Ehle [7]
Lobatto IIIC	$2s-2$	$s-2$	L-stable for all s	Chipman [5]
RK $(s, c = 1)$	$2s-2$	s	L-stable for all s	[This paper]
RK $(s, c > 1/2)$	$2s-2$	s	Strongly A-stable for all s	[This paper]

From Table 1.1, we see that the class of new RK $(s, c = 1)$ methods seems to be more attractive than Lobatto IIIC methods by having the stage order higher. Especially, RK $(s, c > 1/2)$ forms a family of strongly A-stable methods which gives us a freedom on the choice of one collocation point. Several possibilities of exploiting this freedom applied to parallel integrations will be discussed in Section 3 where we report an application of a special class of the new IRK methods to a parallel iteration scheme. This application shows a promising aspect of the IRK methods proposed in this paper. We do not claim that this family of new IRK methods is already accepted as the efficient ODE methods. A further study and application of these methods will be subject of further research.

2. ONE-PARAMETER FAMILY OF IRK METHODS

Let us consider a collocation s-stage implicit Runge–Kutta method (IRK method) based on collocation vector

$$\boldsymbol{c} = (\boldsymbol{c}_{s-1}^T, c_s)^T, \; \boldsymbol{c}_{s-1} = (c_1, \ldots, c_{s-1})^T .$$

For the sake of convenience, we will from now assume that $c_s \neq c_j$ $(j = 1, \ldots, s-1)$ and that c_s is a free parameter abscissa. Furthermore, the subvector $\boldsymbol{c}_{s-1}$ is always the $(s-1)$-dimensional Gauss collocation vector, that is the components c_j, $j = 1, \ldots, s-1$ are the zeros of the shifted Legendre polynomial of degree $s-1$

$$\frac{d^{s-1}}{dx^{s-1}}\left(x^{s-1}(x-1)^{s-1}\right).$$

The resulting s-stage RK (s, c) method is now depending on the free abscissa c_s and will be denoted by RK (s, c_s).

2.1. Order considerations

The results about order of accuracy of the RK (s, c_s) methods are given in the following theorem:

Theorem 2.1. *The RK (s, c_s) method is of stage order $r = s$ and step point order $p = 2s-2$ for any given integer s and real values of c_s (c_s is different from the zeros of the shifted Legendre polynomial of degree $s-1$).*

Proof. Firstly, we prove that the simplifying conditions $C(s)$ and $B(s+v)$ imply the simplifying condition $D(v)$. Secondly, we show that the weights $b_1, \dots, b_{s-1}, b_s$ of the RK(s, c_s) method defined by the simplifying condition $B(s)$ satisfy also the simplifying condition $B(2s-2)$ for any real values of c_s. Then, Theorem 2.1 can be proved by using Butcher's Theorem (cf. e.g. [9, p. 204], [10, p. 75]).

2.2. Stability considerations

Since the s–stage RK $(s,\ c_s)$ method is of collocation type, its rational stability function $R(z)$ has the form (cf. e. g. [10, p. 48], and also [18], [16])

$$R(z) = \frac{M^{(s)}(1) + M^{(s-1)}(1)z + \cdots + M(1)z^s}{M^{(s)}(0) + M^{(s-1)}(0)z + \cdots + M(0)z^s} = \frac{P(z)}{Q(z)} \tag{2.1}$$

where

$$M(x) = \frac{1}{s!}\prod_{i=1}^{s}(x - c_i)\,. \tag{2.2}$$

We can show that the following relations are satisfied

$$|R(\infty)| = \begin{cases} 1 & \text{for } c_s = 1/2 \\ \beta < 1 & \text{for } c_s > 1/2 \\ 0 & \text{for } c_s = 1 \end{cases} \tag{2.3}$$

Basing on the results concerning with the conditions for I–stability of a rational function $R(z) = P(z)/Q(z)$ (cf. [10, Prop. 3.6, p. 44]) by the virtue of Theorem 2.1 and in view of the relation (2.3) we have:

Theorem 2.2. *For any given s, the stability function $R(z)$ of the RK$(s,\ c_s \geq 1/2)$ method is I–stable (c_s is different from the zeros of the shifted Legendre polynomial of degree $s-1$).* ▯

It is noted that the stability function of RK $(s,\ c_s \geq 1/2)$ method is not a Padé approximation to the exponential function. The applications of order stars to a pth–order I–stable rational approximation $R(z)$ to the exponential function e^z reveal that $p \leq 2d_1$, where d_1 is the number of poles of $R(z)$ lying in the positive half complex plane $C^+ := \{z \in C : Re(z) > 0\}$ (cf. [10, Theorem 4.7, p. 58]). From here, it can be shown that the stability function of RK $(s,\ c_s \geq 1/2)$ method has no poles in

$C^- := \{z \in C : Re(z) < 0\}$. By means of Theorem 2.2, Maximum principle, and relation (2.3), we obtain the final theorem about the properties of the family of RK (s, c_s) methods:

Theorem 2.3. *For the stability properties of the family of* $RK(s, c_s)$ *methods, where* c_s *is different from the zeros of the shifted Legendre* $s-1$*, the following assertions hold:*

(i) $RK(s, c_s = 1/2)$ *method is A–stable for any odd values of* s.

(ii) $RK(s, c_s > 1/2)$ *method is strongly A–stable for any* s. *Moreover,* $RK(s, c_s = 1)$ *is L–stable.*

3. AN APPLICATION TO PARALLEL INTEGRATIONS

In this section we consider an application of the new family of RK (s, c_s) methods to the parallel predictor–corrector iteration scheme (PIRK (s, c_s) methods). This iteration scheme is defined exactly the same as PISRK methods proposed in [15]. For a scalar equation it assumes the form

$$\boldsymbol{Y}_n{}^{(0)} = V\boldsymbol{Y}_{n-1}^{(m)} + \boldsymbol{w}y_n, \quad \boldsymbol{Y}_0{}^{(0)} = \boldsymbol{e}y_0 \tag{3.1}$$

$$\boldsymbol{Y}_n{}^{(j)} = \boldsymbol{e}y_n + hAf(\boldsymbol{Y}_n{}^{(j-1)}), \quad j = 1, \ldots, m, \tag{3.2}$$

$$y_{n+1} = y_n + h\boldsymbol{b}^T f(\boldsymbol{Y}_n), \tag{3.3}$$

where the s–by–s matrix V and s–dimensional vector $\boldsymbol{w}$ are determined by order conditions (see also [15]).

The rate of convergence of (3.1) is defined by using the model test equation $y'(t) = \lambda y(t)$ and characterized by the *convergence factor* $\rho(A)$ (cf. [11], [15]). We can exploit the freedom in the choice of the collocation vector abscissa c_s of the corrector RK (s, c_s) for minimizing the convergence factor $\rho(A)$. In this paper we restrict our considerations to the special class of corrector methods RK $(s, c_s = 0)$. Table 3.1 lists the convergence factors for the PIRK $(s, c_s = 0)$ and the PIRK methods proposed in [12]. From this table, we see that the convergence factors of the PIRK $(s, c_s = 0)$ methods are substantially smaller than those of the PIRK methods of the same order.

The numerical experiments have also shown that the PIRK $(s, c_s = 0)$ methods are superior to the PIRK methods of the same order by a speed up factor about two.

Table 3.1. Convergence factors of the pth–order PIRK and PIRK (s, $c_s = 0$) methods

Methods	$p = 4$	$p = 6$	$p = 8$	$p = 10$
PIRK	0.289	0.215	0.165	0.137
PIRK (s, $c_s = 0$)	0.166	0.164	0.141	0.119

4. CONCLUSIONS

In this paper we propose a new family of high order *A*-stable Runge–Kutta processes which seem to be promising numerical methods for ODEs.

The class of *L*-stable RK (s, $c_s = 1$) methods which forms the fourth class of *L*-stable IRK methods in the literature seems to be more attractive than the class of *L*-stable Lobatto IIIC methods by being of higher stage order (cf. Section 1, Table 1.1). We hope that this class of methods would be efficient integrator for stiff ODE problems.

The family of strongly *A*-stable methods RK (s, $c_s > 1/2$) is attractive by having the freedom on the choice of one collocation point. This freedom can be used for constructing parallel diagonally implicit Runge–Kutta methods for stiff problems as in [13]. This subject will be investigated in the forthcoming paper.

A class of parallel predictor–corrector iteration methods PIRK (s, $c_s = 0$) applied to the special class RK (s, $c_s = 0$) of the new RK (s, c_s) methods have better convergence than PIRK methods based on Gauss–Legendre IRK methods.

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