Part II

# NUMERICAL MATHEMATICS

BIT 33 (1993), 620–633.

# OPTIMAL ORDER DIAGONALLY IMPLICIT RUNGE-KUTTA METHODS

A. H. AL-RABEH

*Department of Systems Engineering*
*King Fahd University of Petroleum & Minerals*
*Dhahran-31261 – Saudi Arabia*

**Abstract.**

In this paper, the optimal order of non-confluent Diagonally Implicit Runge-Kutta (DIRK) methods with non-zero weights is examined. It is shown that the order of a $q$-stage non-confluent DIRK method with non-zero weights cannot exceed $q + 1$. In particular the optimal order of a $q$ stage non-confluent DIRK method with non-zero weights is $q + 1$ for $1 \leq q \leq 5$. DIRK methods of orders five and six in four and five stages respectively are constructed. It is further shown that the optimal order of a non-confluent $q$ stage DIRK method with non-zero weights is $q$, for $q \geq 6$.

*AMS Subject Classification:* 65L05.

*Key-words:* Stiff Ordinary Differential Equations, Diagonally Implicit Runge-Kutta methods.

## 1. Introduction.

In this paper, we are concerned with the approximate numerical integration of the $m$-dimensional stiff initial value problem,

$$y' = f(x, y), \qquad y(x_0) = y_0 \tag{1}$$

using a $q$-stage Diagonally Implicit Runge Kutta (DIRK) method:

$$K_i^{(n)} = f\left(x_n + c_i h, h \sum_{j=1}^{i} a_{ij} k_j^{(n)}\right), \quad i = 1(1)q, \tag{2}$$

and,

$$y_{n+1} = y_n + h \sum_{i=1}^{q} b_i k_i^n,$$

where there exists an $s$, $1 \leq s \leq q$, such that $a_{ss} \neq 0$. A $q$-stage DIRK method of order $p$ is referred to by the pair $(q, p)$. DIRK methods have been studied by Norsett

Received February 1992. Revised May 1993.

[14, 17], Crouzeix [9], Alexander [1], Cash [7, 8], Cooper and Safy [10], Al-Rabeh [2, 3, 4], and Dekker at. al [12]. A particular class of DIRK methods for which all the diagonal elements $a_{ii}$, $i = 1(1)q$ of the coefficiënt matrix are equal has received attention as these methods can be implemented efficiently. Optimal methods of orders 2, 3, and 4 in 1, 2, and 3 stages have been derived. However, Alexander [1] has shown that no method of order 5 in 4 stages exists. Norsett [15] conjectured that no $q$ stage DIRK method of order $q + 1$ exists if $q$ is any even number greater than 2.

In this paper we examine the attainable order of the general class of DIRK methods defined by (2). In section two the attainable order of DIRK methods is discussed. In section three certain properties of optimal order DIRK methods are derived. In sections four and five (4, 5) and (5, 6) DIRK methods are constructed, In section six the existence of a (6, 7) DIRK method is examined.

## 2. Attainable Order of DIRK Methods.

Butcher [6] has shown that for any $q \geq 1$, there exists a $q$-stage implicit Runge-Kutta method of optimal order $2q$. For DIRK methods the attainable order is considerably lower. Before examining the problem of attainable optimal order for DIRK methods, we need some preliminary results.

Following Dahlquist et al. [11] we state,

DEFINITION: A DIRK method is non-confluent if all $c_i$, $i = 1(1)q$, are distinct and confluent otherwise.

Following Butcher [5, 6], we shall use the symbols $A$, $B$, $F$, $G$, and $E$ to represent statements about some interesting groups of the order equations.

$A(p)$: $\Phi = 1/\gamma$, whenever $r \leq p$, where $r$ is the order of the elemental weight. (These are all the order equations).

(3) $$B(p):\ \varphi = \sum_{i=1}^{q} b_i = 1,$$

$$[\varphi^{k-1}] = \sum_{i=1}^{q} b_i c_i^{k-1} = \frac{1}{k}, \quad \text{for} \quad k = 1(1)p,$$

(4) $$F(p):\ [{}_2\varphi]_2 = \sum_{i,j=1}^{q} b_i a_{ij} c_j = \tfrac{1}{6},$$

$$[[\varphi]\varphi^{k-3}] = \sum_{i,j=1}^{q} b_i c_i^{k-3} a_{ij} c_j = \frac{1}{2k}, \quad \text{for} \quad k = 4(1)p,$$

(5) $$G(p)\colon\ [_2\varphi^2]_2 = \sum_{i,j=1}^{q} b_i a_{ij} c_j^2 = \tfrac{1}{12},$$

$$[[\varphi^2]\varphi^{k-4}] = \sum_{i,j=1}^{q} b_i c_i^{k-4} a_{ij} c_j^2 = \frac{1}{3k}, \quad \text{for} \quad k = 5(1)p,$$

(6) $$E(p)\colon\ [_2\varphi^{k-2}]_2 = \sum_{i,j=1}^{q} b_i a_{ij} c_j^{k-2} = \frac{1}{k(k-1)}, \quad k = 3(1)p.$$

Using these relationships the following results are stated:

THEOREM (1): *Butcher* [6]
(i) $A(p) = > B(p)$.
(ii) $A(p) = > F(p)$.
(iii) $A(p) = > G(p)$.
(iv) $A(p) = > E(p)$.

Using Theorem (1), the following result is formulated:

THEOREM (2): *A non-confluent (q, p) DIRK method with non-zero weights has an order p that cannot exceed q + 1.*

PROOF: Assume that there exists a non-confluent $(q, q + 2)$ DIRK method with non-zero weights, then $B(q + 2)$, $F(q + 2)$, and $G(q + 2)$.

Set

$$P_i = \sum_{j=1}^{q} a_{ij} c_j - c_i^2/2, \qquad i = 1(1)q.$$

$$T_i = \sum_{j=1}^{q} a_{ij} c_j^2 - c_i^3/3, \qquad i = 1(1)q.$$

then we shall show that $P_i = T_i = 0$, for $i = 1(1)q$.

Consider combining $B(q + 2)$ and $F(q + 2)$, then

$$[_2\varphi]_2 - \tfrac{1}{2}[\varphi^2] = 0,$$

$$[[\varphi]\varphi^{k-3}] - \tfrac{1}{2}[\varphi^{k-1}] = 0, \qquad k = 4(1)q + 2,$$

or, equivalently, writing out in full

$$\sum_{i=1}^{q} b_i P_i c_i^r = 0, \qquad r = 0(1)q - 1.$$

Since the DIRK method is nonconfluent with non-zero weights, then $P_i = 0$ for $i = 1(1)q$.

Note that $P_1 = 0 => c_1 = 0 => T_1 = 0$, also $P_2 = 0 => a_{22} = \frac{c_2}{2}$.

Considering combining equations $B(q+2)$ and $G(q+2)$, then

$$[_2\varphi^2]_2 - \tfrac{1}{3}[\varphi^3] = 0,$$
$$[[\varphi^2]\varphi^{k-4}] - \tfrac{1}{3}[\varphi^{k-1}] = 0, \qquad k = 5(1)q+2,$$

or, writing out in full

$$\sum_{i=1}^{q} b_i T_i c_i^r = 0, \qquad r = 0(1)q-2,$$

but since $T_1 = 0$, then

$$\begin{pmatrix} b_2 & \dots & b_q \\ \cdot & \dots & \cdot \\ \cdot & \dots & \cdot \\ \cdot & \dots & \cdot \\ c_2^{q-2} b_2 & & c_q^{q-2} \end{pmatrix} \begin{pmatrix} T_2 \\ \cdot \\ T_q \end{pmatrix} = 0,$$

and a similar argument leads to,

$$T_i = 0, \quad \text{for} \quad i = 1(1)q,$$

but $T_2 = 0 => a_{22} = \frac{1}{3}c_2$, which contradicts the previous result.

To complete the proof, we need to show that the theorem is true for $q = 1$. This is simple to show, since the one stage DIRK method is the well known midpoint rule which is of order 2.

By considering the $N$-rational approximation to $e^z$, $z \in C$, Norsett and Wolfbrandt [16], have shown that the order of any $q$-stage DIRK method cannot exceed $q + 1$. Their approach is quite different from that presented. It is noted, however, that Norsett and Wolfbrandt [16], do not impose any conditions on the nodes $c_i$'s and the weights $b_i$'s.

## 3. Properties of Optimal DIRK Methods.

As a consequence of Theorem (1), we turn our attention to $q$-stage DIRK methods of order $q + 1$. Following Butcher [5], and Dekker et. al [12], we shall use the symbols $C$, and $D$ to represent some convenient relationships between the coefficients of the DIRK method:

(7) $$C(\xi)\colon \sum_{j=1}^{q} a_{ij} c_j^{k-1} = \frac{1}{k} c_i^k, \quad i = 1(1)q, \quad k = 1(1)\xi,$$

(8) $$D(\xi)\colon \sum_{j=1}^{q} b_j a_{ji} c_j^{k-1} = \frac{1}{k} b_i (1 - c_i^k), \quad i = 1(1)q, \quad k = 1(1)\xi.$$

To help us construct such methods, we shall replace some of the order equations with a much more convenient set of equations.

LEMMA 1: *For any non-confluent* $(q, p)$ *DIRK method, with* $p = q + 1$, *then* $D(1)$.

PROOF: Set

$$d_i = \sum_{j=1}^{q} a_{ji} b_j - (1 - c_i) b_i, \qquad i = 1(1)q.$$

We shall show that $d_i = 0$ for $i = 1(1)q$.

Consider the vector:

$$\underline{u}_i = (1, c_i, \ldots, c_i^{q-1})^T, \qquad i = 1(1)q.$$

Now, if all the $c_i$'s are distinct, then set:

$$\underline{w} = \sum_{i=1}^{q} d_i \underline{u}_i = (\Sigma d_i \ldots \Sigma c_i^{q-1} d_i)^T.$$

For some constants $d_i$, $i = 1(1)q$.

Since the DIRK method used is of order $q + 1$ then $B(q + 1)$ and $E(q + 1)$, using Theorem (1).

Now, consider a typical component of $\underline{w}$, then,

$$w_k = \sum_{i}^{q} c_i^{k-1} d_i = [{}_2\varphi^{k-1}]_2 - [\varphi^{k-1}] + [\varphi^k] = 0,$$

i.e. $\underline{w} = 0$, but since $\underline{u}_i$ are linearly independent for $i = 1(1)q$, then

$$d_i = 0,, \quad \text{for} \quad i = 1(1)q.$$

The set of equations $D(1)$ has the effect of ensuring that all first degree elementary weight have the correct values if the same is true for the other elementary weights.

LEMMA 2: *For a non-confluent* (4, 5) *DIRK method with non-zero weights* $C(2)$.

PROOF: Let $p_i = \sum_{j=1}^{4} a_{ij} c_j - \frac{1}{2} c_i^2, \qquad i = 1(1)q.$

Assume that not all $p_i$, $i = 1(1)q$ vanish, then using the order equations given in Butcher [6], we have

(i) $\sum_{i=1}^{4} b_i p_i = 0,$ (ii) $\sum_{i=1}^{4} b_i c_i p_i = 0,$

(iii) $\sum_{i=1}^{4} b_i c_i^2 p_i = 0,$ (iv) $\sum_{i=1}^{4} b_i p_i^2 = 0,$

For example, to verify (iv), we have,

$$\sum_{i=1}^{4} b_i p_i^2 = \sum_{i=1}^{4} b_i \left( \sum_{j=1}^{4} a_{ij} c_j \right)^2 - \sum_{j=1}^{4} b_i c_i^2 a_{ij} c_j + \tfrac{1}{4} \sum_{i=1}^{4} b_i c_i^4 = \tfrac{1}{20} - \tfrac{1}{10} + \tfrac{1}{20} = 0,$$

Equations (i) to (iv) could be rewritten in matrix form.

$$\begin{pmatrix} b_1 & \dots & b_4 \\ c_1^2 & \dots & . \\ c_1 b_1 & \dots & . \\ p_1 b_1 & & p_4 b_4 \end{pmatrix} \begin{pmatrix} p_1 \\ p_2 \\ p_3 \\ p_4 \end{pmatrix} = 0,$$

Since not all the $p_i$'s vanish, and the DIRK method is nonconfluent with non-zero weights, then:

(9) $$p_i = tc_i^2 + uc_i + v, \qquad i = 1(1)4,$$

for some constants $t$, $u$ and $v$, (not all zero).

Now, substitute (9) into (i), (ii) and (iii), and using the order equations,

$$t/3 + u/2 + v = 0,$$

$$t/4 + u/3 + v/2 = 0,$$

$$t/5 + u/4 + v/3 = 0.$$

Thus, $t = u = v = 0$, a contradiction. Therefore, $P_i = 0$, for $i = 1(1)q$.

REMARK: Lemma 2 can be generalized to any $(q, q+1)$ DIRK method, where $q > 4$, using

(10) $$\sum_{i=1}^{q} b_i c_i^{k-3} p_i = 0, \qquad k = 3(1)q+1,$$

which follows from combining $B(q+1)$ together with $F(q+1)$.

LEMMA 3: *For a non-confluent* (5, 6) *DIRK method with non-zero weights, and not all $T_i$'s are zero where*

(11) $$T_i = \sum_{j=1}^{q} a_{ij} c_j^2 - \frac{c_i^3}{3}, \qquad i = 1(1)q.$$

Then, $D(2)$,

PROOF: Set

(12) $$s_i = \sum_{j=1}^{q} b_j c_j a_{ji} - \tfrac{1}{2} b_i (1 - c_i^2); \qquad i = 1(1)q.$$

Then, using the order equations we have the following:

Equations (i) yo (iv) could be rewritten in matrix form.

(i) $\sum_{i=1}^{q} s_i = 0,$ (ii) $\sum_{i=1}^{q} s_i c_i = 0,$ (iii) $\sum_{i=1}^{q} s_i c_i^3 = 0,$

(iv) $\sum_{i=1}^{q} s_i c_i^3 = 0,$ (v) $\sum_{i=1}^{q} s_i T_i = 0.$

Equations (i), (ii), and (iii) are easily verified using the order equations, given in Butcher [6]. Furthermore,

$$\text{(iv)} \sum_{i=1}^{q} s_i c_i^3 = \sum_{i,j=1}^{q} b_j c_j a_{ji} c_i^3 - \tfrac{1}{2}\left(\sum_{i=1}^{q} b_i c_i^3 - \sum_{i=1}^{q} b_i c_1^5\right)$$

$$= [[\varphi^3]\varphi] - \tfrac{1}{2}\{[\varphi^3] - [\varphi^5]\} = 0, \text{ using Theorem (1),}$$

$$\text{(v)} \sum_{i=1}^{q} T_i s_i = \sum_{i,j,k=1}^{q} b_i c_i a_{ij} a_{jk} c_k^2 - \tfrac{1}{2}\left(\sum_{i,j=1}^{q} b_i a_{ij} c_j^2 - \sum_{i,j=1}^{q} b_i c_i^2 a_{ij} c_i^2\right)$$

$$+ \tfrac{1}{3}\sum_{i,j=1}^{q} b_i c_i a_{ij} c_j^3 + \tfrac{1}{6}\left\{\sum_{i=1}^{q} b_i c_i^3 - \sum_{i=1}^{q} b_i c_i^5\right\}$$

$$= [[_2\varphi^2]_2\varphi] - \tfrac{1}{2}\{[_2\varphi^2]_2 - [[\varphi^2]\varphi^2]\}$$

$$-\tfrac{1}{3}[[\varphi^3]\varphi] + [\tfrac{1}{6}\{[\varphi^3] - [\varphi^5]\} = 0.$$

Using Theorem (1) and the order equations.

Equations (i)–(v) give

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ c_1 & c_2 & c_3 & c_4 & c_5 \\ c_1^2 & . & . & . & . \\ c_1^3 & . & . & . & . \\ T_1 & . & . & . & T_5 \end{pmatrix} \begin{pmatrix} s_1 \\ . \\ s_5 \end{pmatrix} = \underline{0}$$

If the determinant of the matrix is zero, and the method is nonconfluent then:

$$T_i = \lambda c_i^3 + \mu c_i^2 + \delta c_i + \sigma, \qquad i = 1(1))q \tag{13}$$

for some constants $\lambda$, $\mu$, $\delta$ and $\sigma$, (not all zero). Using the order equations we have:

(14) (a) $\sum_{i=1}^{q} b_i T_i = 0,$ (b) $\sum_{i=1}^{q} b_i c_i T_i = 0,$ (c) $\sum_{i=1}^{q} b_i c_i^2 T_i = 0.$

Substitute $T_i$ given by (13) in (a), (b) and (c), we have:

$$(1/4)\lambda + (1/3)\mu + (1/2)\delta + \sigma = 0$$

$$(1/5)\lambda + (1/4)\mu + (1/3)\delta + (1/2)\sigma = 0$$

$$(1/6)\lambda + (1/5)\mu + (1/4)\delta + (1/3)\sigma = 0$$

Now, from the generalization of Lemma 2:

$$c_1 = 0 = T_1 = 0 = > \varphi = 0, \quad \text{but} \quad \sigma = 0 = > \lambda = \mu = \delta = 0.$$

which contradicts the requirement of the Lemma. Hence, $s_i = 0$ for $i = 1(1)q$.

Alexander [1] and Norsett [14], constructed DIRK methods of optimum order for $q = 1, 2$ and 3. Using the previous Lemmas, (4, 5) and (5, 6) DIRK methods will be constructed. Moreover, the existence of a (6, 7) DIRK method will be investigated.

## 4. (4, 5) DIRK Methods.

For a fifth order DIRK method we need to satisfy a set of 17 order equations (Butcher [6]). Alternatively, consider the following equations:

(i) $B(5)$, (ii) $C(2)$, (iii) $D(1)$, (iv) $\sum_{i,j=1}^{4} b_i c_i a_{ij} c_j^2 = \frac{1}{15}$.

The original order equations can be replaced with the much simpler equations (i) to (iv). As an example, we can see that elementary weights of degree one, and elementary weights of the form, $[[\varphi]\varphi_1 \ldots \varphi_s]$ are satisfied if (i) to (iv) are true. For example:

$$\begin{aligned}
[_4\varphi]_4 &= \sum_{i,j,k,l}^{q} b_i a_{ij} a_{jk} a_{kl} c_1 \\
&= \tfrac{1}{2} \sum_{i,j,k}^{q} b_i a_{ij} a_{jk} c_k^2, \text{ using (ii)} \\
&= \tfrac{1}{2} \left\{ \sum_{j,k}^{q} b_j a_{jk} c_k^2 - \sum_{j,k}^{q} b_j c_j a_{jk} c_k^2 \right\}, \text{ using (iii)} \\
&= \tfrac{1}{2} \left\{ \sum_{j=1}^{q} c_j^2 b_j - \sum_{j=1}^{q} c_j^3 b_j - \tfrac{1}{15} \right\}, \text{ using (iii) and (iv)} \\
&= \tfrac{1}{20} \text{ using (i).}
\end{aligned}$$

Thus, the elementary weight $[_4\varphi]_4$ has the correct value. The rest of the order equations can be treated similarly.

Equations (i) to (iv) represent a set of 14 equations which are more convenient to solve than the original 17 order equations. It is simple to verify that,

(v) $\sum_{i=1}^{4} b_i T_i = 0$, (vi) $\sum_{i=1}^{4} b_i c_i T_i = 0$,

where $T_i$ is as defined by (11).

Solving the set of 14 equations and using (v) and (vi) results in a two parameter family of DIRK methods.

*Special Choice of Parameters.*

Set $a_{22} = a_{33} = a_{44}$, then, $a_{33} = \frac{1}{2}c_2 = 1 - c_4$, i.e. $c_2 = 2(1 - c_4)$, and $a_{33} = a_{44} = > c_4^3 - 2c_4^2 + \frac{5}{4}c_4 - \frac{7}{30} = 0$

The solution of the above equation results in exactly three DIRK methods, they are:

| | | | | |
|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 |
| 0.2180780182 | 0.1090390091 | 0.1090390091 | 0 | 0 |
| 0.5545195045 | 0.0177359481 | 0.4277445474 | 0.1090390091 | 0 |
| 0.8909609909 | 0.1173343519 | 0.2044057169 | 0.4601819131 | 0.1096390091 |
| | 0.0707307044 | 0.3078968440 | 0.3589454736 | 0.2624269779 |

| | | | | |
|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 |
| 0.463866737 | 0.2319333685 | 0.2319333658 | 0 | 0 |
| 0.6159666843 | 0.2830468765 | 0.1009864392 | 0.2319333685 | 0 |
| 0.7680666315 | 0.2181834746 | 0.5195503629 | −0.2016005745 | 0.2319333685 |
| | 0.1269880164 | 1.1744777572 | −1.2277758135 | 0.9263100398 |

| | | | | |
|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 |
| 1.3180552448 | 0.6590276224 | 0.6590276224 | 0 | 0 |
| 0.8295138112 | 0.3242171755 | −0.1537309866 | 0.6590276224 | 0 |
| 0.3409723776 | −0.0474436927 | 0.1185096734 | −0.3891212254 | 0.6590276224 |
| 0.1059840102 | 0.0020003972 | 0.3954847537 | 0.3954847537 | 0.4965308389 |

Alexander [1], showed that there are no DIRK methods of order 5 in 4-stages if $a_{ii} = \alpha$ for $i = 1(1)4$, hence one advantage of allowing unequal diagonal elements is the achievement of higher order.

## 5. (5, 6) DIRK Methods.

The construction of DIRK methods of higher order ($p > 5$) becomes increasingly difficult; for example, to achieve order six, we need to satisfy a set of 37 algebraic equations, a difficult task, but again using Lemma, 1, 2 and 3 these equations could be reduced to a more manageable set of 22 simple algebraic equations as follows

(i) $B(6)$ (ii) $C(2)$ (iii) $D(1)$ (iv) $D(2)$ (v) $\sum_{i=1}^{5} b_i c_i^2 a_{ij} c_j^2 = \frac{1}{18}$.

The analysis of the (4, 5) DIRK method indicates that if (i) to (iv) are true, then the first 17 order equations are satisfied. Note that equation (iv) in the (4, 5) case is not included in our set since,

$$\sum_{i,j=1}^{5} b_i c_i a_{ij} c_j^2 = \tfrac{1}{2}\left\{\sum_{i,j-1}^{5} b_j c_j^2 - b_j c_j^4\right\} \text{using (iv)}$$
$$= \tfrac{1}{2}\{\tfrac{1}{3} - \tfrac{1}{5}\} = \tfrac{1}{15}, \text{ using (i).}$$

It remains to show that the order six elementary weights are also satisfied. Overall, we have some 20 elementary weights of order six, See Butcher [6].

Recall that (iii) = > all first degree elementary weights have the correct value if the same is true for all the other elementary weights. Thus, we only need to concern ourselves with elementary weights of order 6 and degree $>1$.

Similarly, we do not need to concern ourselves with elementary weights of the form $[[\varphi], \varphi_1 \ldots \varphi_s]$ since it was shown that if (ii) is true, then these elementary weights have the correct value.

The remaining equations, excluding (i) and (v), are as follows:

a. $[[\varphi][_2\varphi]_2\varphi^2] = \sum_{i,j,k}^{5} b_i c_i^2 a_{ij} a_{jk} c_k = \tfrac{1}{36}$;

b. $[[[\varphi]\varphi]\varphi] = \sum_{i,j,k}^{5} b_i c_i a_{ij} c_j a_{jk} c_k = \tfrac{1}{48}$;

c. $[[\varphi^3]\varphi] = \sum_{i,j}^{5} b_i c_i a_{ij} c_j^3 = \tfrac{1}{24}$;

d. $[[_3\varphi]_3\varphi] = \sum_{i,j,k,l}^{5} b_i c_i^2 a_{ij} a_{jk} c_1 = \tfrac{1}{144}$;

e. $[[_2\varphi^2]_2\varphi] = \sum_{i,j,k}^{5} b_i c_i a_{ij} a_{jk} c_k^2 = \tfrac{1}{72}$.

It is a relatively simple task to show that equation (iv) assuming (i) and (v) implies equations b, c, d, and e, for example b:

$$[[[\varphi]\varphi]\varphi] = \sum_{i,j,k}^{5} b_i c_i a_{ij} c_j a_{jk} c_k$$
$$= \tfrac{1}{2} \sum_{j,k}^{5} b_j c_j a_{jk} c_k$$
$$= \tfrac{1}{2}\left\{[[\varphi]\varphi] - \tfrac{1}{2}\sum_j b_j c_j^5\right\} \text{ using (ii)}$$
$$= \tfrac{1}{2}\{\tfrac{1}{8} - \tfrac{1}{12}\}, \text{ (using (ii))}$$
$$= \tfrac{1}{48}, \text{ (the correct value).}$$

We have shown that if the 22 conditions given by equations (i) to (v) hold, then the original 37 order equations are satisfied.

The order equations yield a two parameter family of DIRK methods with the following interesting relationships among the coefficients:

$$c_5 = 1, \quad a_{55} = 0, \quad \text{and} \quad a_{44} = \tfrac{1}{2}(1 - c_4).$$

EXAMPLE: Set $c_2 = \frac{1}{4}$, and $c_4 = \frac{3}{4}$, then the following DIRK method is of order 6.

| | | | | | |
|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 |
| 1/4 | 1/8 | 1/8 | 0 | 0 | 0 |
| 1/2 | −1/12 | 2/3 | −1/12 | 0 | 0 |
| 3/4 | 1/8 | 1/4 | 1/4 | 1/8 | 0 |
| 1 | 0 | 4/7 | −1/7 | 4/7 | 0 |
| | 7/90 | 16/45 | 2/15 | 16/45 | 7/90 |

Unfortunately, the above DIRK is not $A$-stable.

As a result of Theorem (2), and the construction of DIRK methods of orders 2, 3, ... 6 in 1, 2, ... 5 stages respectively, we state the following result:

THEOREM (3): *The optimal order of a non-confluent $(p, q)$ DIRK method with non-zero weights is $q + 1$, for $q \leq 5$.*

## 6. The Non-existence of a (6, 7) DIRK method.

In this section we investigate the existence of a (6, 7) DIRK method.

THEOREM (4): *For the non-confluent class of DIRK methods with non-zero weights, there is no DIRK method of order 7 in six stages.*

PROOF: Let

$$T_i = \sum_{i=1}^{6} a_{ij} c_j^2 - \tfrac{1}{3} c_i^3, \qquad i = 1(1)6. \tag{14}$$

For a DIRK method of order 7, the following equations (i) to (v) are necessary conditions:

(i) $\sum_{i=1}^{6} b_i T_i = 0$, (necessary for order 4).

(ii) $\sum_{i=1}^{6} b_i c_i^2 T_i = 0$, (necessary for order 6).

(iii) $\sum_{i=1}^{6} b_i c_i^2 T_i = 0$, (necessary for order 6).

(iv) $\sum_{i=1}^{6} b_i c_i^3 T_i = 0$, (necessary for order 7).

(v) $\sum_{i=1}^{6} b_i T_i^2 = 0$, (necessary for order 7).

It is relatively simple to verify the above equations, for example:

$$\text{(iv)} \quad \sum_{i=1}^{6} b_i c_i^3 T_i = \sum_{i,j}^{6} b_i c_i^3 a_{ij} c_j^2 - \tfrac{1}{3} \sum_{i=1}^{6} b_i c_i^6$$
$$= [[\varphi^2]\varphi^3] - \tfrac{1}{3}[\varphi^6] = 0, \text{ using Theorem (1).}$$

We shall show that the only possibility is $T_i = 0$, $i = 1(1)6$, which leads to a contradiction.

Lemma 2 = $> c_1 = 0$, thus $T_1 = 0$.

Hence, equations (i) to (v) give:

$$\begin{pmatrix} b_2 & b_3 & b_4 & b_5 & b_6 \\ c_2 b_2 & c_3 b_3 & . & . & . \\ c_2^2 b_2 & . & . & . & . \\ c_2^3 b_2 & . & . & . & . \\ T_2 b_2 & . & . & . & . \end{pmatrix} \begin{pmatrix} T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \end{pmatrix} = \underline{0}$$

CASE 1: det| | $\neq 0$, then: $T_i = 0$, $1 = i(1)6$.

CASE 2: det|.| $= 0$, since the DIRK method is nonconfluent with non-zero weights then:

$$T_i = \lambda c_i^3 + \mu c_i^2 + \delta c_i + \sigma, \qquad i = 2(1)6$$

for some real constants, $\lambda$, $\mu$, $\delta$ and $\sigma$.

Using (i), (ii), (iii) and (iv), we have,

$$\begin{pmatrix} 1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{5} \\ \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \frac{1}{6} \\ \frac{1}{4} & \frac{1}{5} & \frac{1}{6} & \frac{1}{7} \end{pmatrix} \begin{pmatrix} \lambda \\ \mu \\ \delta \\ \sigma \end{pmatrix} = \underline{0}$$

Hence, $\lambda = \mu = \delta = \sigma = 0$ and, $T_i = 0$, $i = 1(1)6$.

Now, $T_2 = 0$ implies that $a_{22} = \frac{1}{3} c_2$ but Lemma 2 = $> a_{22} = \frac{1}{2} c_2$, as $c_2 \neq c_1 = 0$, hence we have a contradiction.

REMARK: Clearly, the approach of the previous theorem can easily be generalized.

THEOREM (5): *Among the class of non-confluent DIRK methods with non-zero weights there are no methods of order* $q + 1$ in q-stages, for $q \geq 6$

PROOF: Similar to Theorem (4), since

(i) $\sum_{i=1}^{q} b_i c_i^k T_i = 0, k = 0(1)q - 3$, and

(ii) $\sum_{i=1}^{q} b_i T_i^2 = 0$, (true for order $\geq 7$).

The above equations can be verified using $B(q + 1)$ and $G(q + 1)$.

Equations (i) and (ii) will give us a $q - 1$ equation for the $(q - 1)$ quantities $T_2, \ldots, T_q$ then we can proceed in exactly the same manner as in the previous theorem.

## 7. Conclusion.

In this paper, the optimal order of non-confluent Diagonally Implicit Runge-Kutta (DIRK) methods with non-zero weights was examined. It was shown that the order of a $q$-stage DIRK method cannot exced $q + 1$. In particular the optimal order of a $q$-stage DIRK method is $q + 1$ for $1 \leq q \leq 5$. DIRK methods of orders five and six in four and five stages respectively were constructed. It was further shown that the optimal order of a $q$-stage DIRK method is $q$, for $q \geq 6$. The results are summarized in the following table:

Table: *DIRK Methods for Optimal Order* $(q, p^*)$.

| No. of Stages $q$ | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| Optimal Order $p^*$ | 2 | 3 | 4 | 5 | 6 | 6 |

## Acknowledgement.

The author would like to acknowledge the support provided by the King Fahd University of Petroleum and Minerals. The author is especially grateful for the comments of an anonymous referee which have led to significant improvements in the paper.

## REFERENCES

1. R. Alexander, *Diagonally Implicit Runge-Kutta methods for stiff ODE's*, SIAM J. of N.A. 14, (1977), 1006–1021.
2. A. Al-Rabeh, *A note on the Enright updating technique*. Comp. & Maths with Appls. 10, (1984), 405–411.
3. A. Al-Rabeh, *Embedded DIRK Methods for the Numerical Integration of Stiff ODE's*, Journal of Comp. Math. 21, No. 1, (1987), 373–379.
4. A. Al-Rabeh, *A variable parameter DIRK algorithm for the numerical integration of stiff systems of ODE's*, J. Comp. Math. with applc 13, No. 4, (1987), 373–379.
5. J. C. Butcher, *Implicit Runge-Kutta processes*. Math. Comp. 18, (1964), 50–64.
6. J. C. Butcher, *The numerical analysis of ordinary differential equations*, John Wiley, (1987).
7. J. R. Cash, *Diagonally implicit Runge-Kutta formulae with error estimate*, Journ. Inst. Math. & Applics. 24, (1979), 293–301.
8. J. R. Cash, J. R., and Leim, C. B., *On the design of a variable order, variable step diagonally implicit Runge-Kutta algorithm*, J. Inst. Maths. & Applics. 26, (1980), 87–98.
9. M. Crouzeix, *On the approximation of ordinary differential equations using Runge-Kutta methods*, Thesis, Paris (1975).
10. G. J. Cooper, and A. Safy, *Semi-explicit A-Stable Runge-Kutta methods*, Maths. of Comp. 33, (1979), 541–556.
11. G. Dahlquist, R. Jeltsch, *Generalized disks of contractivity for explicit Runge-Kutta methods*, Report TRITA-NA-7906. Dept. of Comp. Sci., Roy. Inst. of Techn., Stockholm (1979).
12. J. Dekker, J. Verwer, *Stability of Runge-Kutta methods for stiff nonlinear differential equations*, North-Holland, (1984).
13. E. Hairer, S. P. Norsett, G. Wanner, *Solving Ordinary Differential Equations I: Nonstiff Problems*, Springer-Verlag, (1987).
14. S. P. Norsett, *Semi-explicit Runge-Kutta methods*, Math. Dept. University of Trondheim, Reprint No. 6/74, (1974).
15. S. P. Norsett, *One step methods of Hermite type for numerical integration of stiff systems*, BIT, 14, (1974), 63–77.
16. S. P. Norsett, and A. Wolfbrandt, *Attainable order of rational approximation to the exponential function with only real poles*, BIT 17, (1977), 200–208.
17. S. P. Norsett, P. G. Thomsen, *Embedded SDIRK methods of basic order three*, BIT 24, (1984), 634–646.