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GENERALIZED RUNGE-KUTTA SCHEMES
A GLOBAL APPROACH TO THEIR PARAMETER DEFINING EQUATIONS

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November 6, 1969

ABSTRACT

The problem of obtaining schemes for the numerical solution of
\[ D^p x = x \circ \xi, \quad x \in \mathbb{R} \to \mathbb{R}^n, \] and \( \xi = (D^{p-1} x, \ldots, x) \), is treated. Scheme definitions are provided that include the classical Runge-Kutta and finite difference methods and are, at the same time, generalizations that provide schemes outside this class. A global view of the scheme generation problem is provided by developing a formalism that makes use of differentials after the fashion of Butcher [3]. It is shown that all basic results can be obtained from one definition.
I. INTRODUCTION

We consider the generation of numerical integration schemes for the following n-th order system of p-th order ordinary differential equations,

\[ D^p x = X \circ \xi \]
\[ \xi(a) = b \]

where \( x \in \mathbb{R} \rightarrow \mathbb{R}^n \), \( \xi = (D^{p-1} x, \ldots, x) \in \mathbb{R} \rightarrow \mathbb{R}^{nxp} \), \( X \in \mathbb{R}^{nxp} \rightarrow \mathbb{R}^n \), \( b \in \mathbb{R}^{nxp} \), \( a \in \mathbb{R} \), \( R \) is the real line, \( \mathbb{R}^{nxp} \) and \( \mathbb{R}^n \) are real \( nxp \) and \( n \)-dimensional vector spaces. Scheme definitions are provided that include the classical Runge-Kutta (RK) and finite difference (FD) schemes and also more recent schemes such as those given by Butcher [1, 2], where use is made of off-step points. They also include generalized Runge-Kutta schemes (GRK). Using the concept of differentials [3], a mathematical formalism is developed that leads to an overall global view of the scheme generation problem. It is shown that all basic results can be obtained from one recursive definition of a generic operator \( Y \) and the generic \( z \) and \( y \) which lie in its domain and range.

The schemes considered are precisely defined in Section III. They can, however, be loosely described as follows. Given an interval of integration, we have, or will construct in a manner described below, a set of approximations \( \xi_i \) to the true solution \( \xi(t_i) \). We also have, or can obtain, the function values \( X_i = X(\xi_i) \). The schemes are defined by saying that any approximation is a linear combination of these quantities.
\begin{equation}
\xi_1 = \sum \alpha_j \xi_j + \sum \beta_j x_j.
\end{equation}

Since nothing has been said about the accuracy of the approximations or the range of the index sets, (1.2) includes both (RK) and (FD) schemes and generalizations of these schemes.

It is the purpose of this paper to derive expressions that define the parameters $\alpha, \beta$ in (1.1). This is done in such a manner that for a particular scheme these expressions may be written down directly and, at the same time, a global view is obtained of the structure of the expressions for all schemes defined by (1.2).

In order to effect the derivation, we define approximations $\zeta \in R \rightarrow R^{n \times p}$, approximations $\xi_1 \in R^{n \times p}$ obtained from a CRK scheme, and a generic set of symbols $z, y$ along with a generic operator $Y$. Using the generic $z, y, Y$, we obtain weighted differentials $W$, derivative harmonics $\alpha$, differentials $A$, weighted polynomials $\Phi$, elementary polynomials $\Gamma$, polynomial weights $\gamma$, product coefficients $\pi$, generalized RK harmonics $H$, and approximation harmonics $\psi$.

Letting $\alpha$ represent the derivative harmonics, it is shown that the derivatives of $\zeta$ can be written as $\Sigma \alpha_i \Phi_i$, Theorem 1. Theorem 2 shows that $D^{i-1}(X \circ \xi) = \Sigma \alpha_i A_i$. We are able to factor $W = \Phi A$ by means of Theorem 3. Using the results of Theorem 4, a general factorization theorem for the generic $z$, we obtain from Theorem 5 that $\alpha \Phi = \alpha \gamma \Gamma = \pi \Gamma = H$. It is then possible to show that the parameter defining equations for all approximations $\xi_1$ have the general form $\Sigma H_1 = \beta \theta^j / j!$ where on the left side there appear the CRK harmonics and on the right side the Taylor harmonics of the exact solution $\xi(\theta)$ times its derivative harmonic.
It is then shown that any GRK approximation can be written as 
\[ \xi_1 = \sum \psi_i A_i \] where the \( \psi_i \) are approximation harmonics; it is this representation that is probably most useful in practice.

The work presented here can be considered to be an extension of the works of Butcher [3], Ceschino-Kuntzmann [4], and R. DeVogelaere [6]. Butcher's results were the principal inspiration for the recursive definition that generates all the differentials and their associated harmonics. The work of Ceschino-Kuntzmann has suggested the form of the scheme definition and has also shown what the results should look like. Professor DeVogelaere has provided not only a concise, precise notation without which it would have been difficult to obtain the necessary expansions, but also his work in RK schemes has furnished a good starting point for the more general formulation given here.

The results presented are a part of the author's thesis [5].
II. NOTATION

In the following work, a rather concise notation will be used and some conventions will be adhered to. The quantities used are usually functions which map from the real line \( \mathbb{R} \) into a vector space; for example \( \xi \in \mathbb{R} \to \mathbb{R}^{\times^2} \). The components are denoted using brackets and the argument using parenthesis. Thus, \( \xi(t)[m] \), or equivalently \( \xi[m](t) \), is the value in \( \mathbb{R}^{\times^2} \) of the \( m \)-th component of \( \xi \) evaluated at \( t \). We are consistent with the use of the parenthesis and brackets. Lower case subscripts and superscripts denote the \( i \)-th element in a set of like elements. As exceptions, we have \( \xi^p \) as the \( p \)-th derivative and \( \theta^j \) as the \( j \)-th power. Upper case subscripts never denote the \( n \)-th element, but instead, the domain of definition of the arguments. We thus use

\[
\begin{align*}
x_N &\in (N \times \mathbb{R}) \to \mathbb{R}, \quad x_N[i](t) = x_N(t)[i] = x(t)[i] \\
D^p x_N[i](t) &= D^p x_N(t)[i] = (D^p x)(t)[i] \\
\xi_L[i](t) &= \xi_L(t)[i] = \xi(t)[i] \\
(X \ast \xi)_N[i](t) &= (X \ast \xi)_N(t)[i] = (X \ast \xi)(t)[i] = X(\xi(t))[i].
\end{align*}
\]

It is also quite useful to carry through the convention of summing on repeated index sets in the following manner. Let

\[K_{LN} \in (L \times N) \to \mathbb{R}\]

that is, a matrix with values \( K_{LN}[m,i] \), \( m \in L, i \in N \). We write

\[
W_L[m](t) = W_L(t)[m] = K_{LN}[m] \cdot T_N(t) = \sum_{i \in N} K_{LN}[m,i] \cdot T_N[i](t).
\]

This can be written as
\[ W_L[m] = K_{LN}[m] \cdot T_N \]

\[ W_L = K_{LN} T_N \]

\[ W_L(t) = K_{LN} \cdot T_N(t) \]

\[ W = K_{LN} T_N \]

which gives a consistent set of notation.

The Taylor's series is used repeatedly in the derivation and it is
concisely represented as

\[ (2.3) \quad X \circ (u + v) = X \circ u + \sum_{s=1}^{1} \frac{1}{s!} (D_{L_1 \ldots L_s} X \circ u) v_{L_1} \ldots v_{L_s} \]

where repeated index sets are summed over,

\[ D_{L_1 \ldots L_s}[m_1, \ldots, m_s] X = \frac{\partial X}{\partial x_{m_1} \ldots \partial x_{m_s}} \]

and

\[ m_i \in L_i = \{1, \ldots, m\} \quad \text{for} \quad i = 1, 2, \ldots, s. \]

Use is made of matrices \( I_{LN}^{(k)} \) that are defined as

\[ (2.4) \quad I_{LN}^{(k)}[m,i] = \delta_{m,i+k} \]

where

\[ m \in L = \{0, 1, \ldots, r \times \phi - 1\} \]

\[ i \in N = \{0, 1, \ldots, n - 1\} \]

\[ k \in P = \{0, 1, \ldots, p - 1\} \]

and \( \delta \) represents the Kroneker delta.

The small center circle, \( \circ \), is used for the usual composition, of a
function or an operator; whereas, the dot, \( \cdot \), signifies multiplication.
It is implicitly assumed that if an operator such as

\[ C_{N_0, N_1}^{(r_0, k_1)} = D^{r_0} \left( D_{L_1} X \circ u \right)_{N_0} L_{L_1} L_{N_1}^{(k_1)} \]

operates on an element in \( R \rightarrow R^n \) such as \( \eta \), then we write \( C_{N_0, N_1}^{(r_0, k_1)} \eta_{N_1} \) and actually carry out the implied summation on repeated indices. Some care must be given to the interpretation of the results. A fuller discussion and examples can be found in [5].
III. GENERALIZED RK METHODS FOR SYSTEMS OF p-th ORDER ORDINARY DIFFERENTIAL EQUATIONS

The general initial value problem considered can be written as

$$D^p x(t)[j] = x(..., D^{p-1} k x(t)[i], ...) [j]$$  \hspace{1cm} (3.1)

$$D^{p-1} k x(0)[i] = a_L[m]$$

where

$$i, j \in \mathbb{N} = \{0, 1, ..., n - 1\}$$

$$k \in \mathbb{P} = \{0, 1, ..., p - 1\}$$

$$m \in \mathbb{L} = \{0, 1, ..., m \times \mathbb{P} - 1\}.$$

The dimension of $x$ is $n$, the order of the differential equation is $p$, and given $m \in \mathbb{L}$, $i$ and $k$ are defined as

$$k = m \div n$$

$$i = m - k \times n$$

where $\div$ is used to denote an integer divide. If $\xi$ is defined as

$$\xi(t)[m] = D^{p-1} k x(t)[i],$$

then (3.1) can be written as

$$D^p x_N = (X \circ \xi)_N$$

$$\xi_L(0) = a_L.$$

We now proceed to define functions $\zeta \in \mathbb{R} \rightarrow \mathbb{R}^{n \times p}$ using the notation

$$\zeta[m] = \zeta^{(k)}[i], m = i + kn \text{ where } i \in \mathbb{N} \text{ and } k \in \mathbb{P}. \text{ Also, let } \phi = \xi_L \in \mathbb{R} \rightarrow \mathbb{R},$$
with $I(t) = t$, and for any function $y$ define $y_1 = y \circ \phi_1$ where it is implicitly assumed that $\theta_1 \in \mathbb{R}$. The approximations are then defined by:

**Definition 1:**

$$\xi_i \in \mathbb{R} \to \mathbb{R}^n \times \mathbb{R}$$

is an approximation if, and only if

$$\xi_i = u_i + \eta_i$$

where

$$u^{(k)}_i = \sum_{r=0}^{l+k} \frac{(\theta_i I)^r}{r!} d^{p-1-k+r}x(0)$$

$$\eta^{(k)}_i = \sum_{r=l+k}^{\infty} \frac{1}{(r+1)!} \frac{(r+1)!}{(r-k)!} d^{r-k} \xi(0)$$

$$g^{(k)}_i = \sum_{j, k_0} g^{(k)}_{ij} \eta^{(k_0)} + \sum_{j} f^{(k)}(X \circ \xi_j)$$

where $k, k_0 \in \mathbb{P} = \{0, \ldots, p-1\}$; $g^{(k)}_{ij}, f^{(k)}_{ij} \in \mathbb{R}$ are constants; $\xi_i, u_i, \eta_i$ are $\mathbb{R} \to \mathbb{R}^n$; $\xi_i = \xi \circ \phi_i$, $u_i = u \circ \phi_i$, $\eta_i = \eta \circ \phi_i$, $\delta_{ir} = \delta \circ \phi_i$ and $\mathbb{I} \in \mathbb{R} \to \mathbb{R}$ such that $I(t) = t$.

In the following work, we shall, occasionally, omit the $r$ when referring to $\delta$ and $f$. It should never be forgotten that such a dependence exists, especially when changing the range over which that index is summed.

We next define quantities $\xi_i \in \mathbb{R}^n \times \mathbb{R}$ which are to be considered as approximations to the true solution $\xi(\theta_1)$.

**Definition 2:**

$\xi_i$ is said to be an approximation obtained by means of a generalized RK scheme if, and only if

$$\xi^{(k)}_i = \sum_{j, k_0} g^{(k)}_{ij} \xi^{(k_0)}_{j_1} + \sum_{j} s^{(k)}_{ij} X(\xi_{j_2})$$

when $X \in \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$ is that of (3.1), $g$ and $a$ are elements of $\mathbb{R}$, and $\xi_j$ is an approximation obtained in the same way.

Given a suitable choice of parameters $g$ and $f$, the approximation $\xi$
will reduce to the vector $\xi = (D^{p-1}x, \ldots, x)$ derived from the true solution $x$ of (3.1) or it will reduce to the GRK approximation $\xi_{i}^{(k)}$ defined in (3.6). These results are summarized as

**Property 1:**

If $\xi_{i}$ is an approximation defined by (3.5) and if $x$ is a solution to (3.4), then $\xi_{i}(1) = \xi(\theta_{i}) = \xi(\theta_{i})$ provided that $g_{ik_{o}j}^{(k)} \equiv 0$ and

\[
\tau_{ik_{r}}^{(k)} = 0, \quad i \neq j
\]

\[
\tau_{ik_{r}}^{(k)} = (r-k)! \frac{\vartheta_{i}^{k+1}}{(r-1)!}
\]

**Property 2:**

If $\xi_{i}$ is an approximation defined by (3.5) and if $\xi_{i}$ is a GRK approximation defined by (3.6), then $\xi_{i}(1) = \xi_{i}$ provided the parameters $g_{ik_{o}j}^{(k)}$, $f_{ik_{r}}^{(k)} = a_{i,j}^{(k)}$ common to both approximations satisfy conditions referred to here as Conditions A.

Property 1 is easily arrived at by writing out $\xi_{i}$ explicitly using the definitions of $\eta_{i}$ and $S_{i,j}$ as given in (3.5) and then substituting the above values of $g$ and $f$. This leads to

\[
(3.7) \quad \xi_{i}^{(k)}(\theta_{i}I) = u^{(k)}(\theta_{i}I) + \sum_{r=k+1}^{\infty} \frac{(\theta_{i}I)^{r+1}}{(r+1)!} D^{-k}(X \circ \xi)(0).
\]

On the other hand, $D^{p}x = X \circ \xi$ where $\xi = u + v$ and $v$ is defined as

\[
v^{(k)} = \sum_{r=k+1}^{\infty} \frac{D^{r+k+r}x(0)}{(r+1)!}
\]

Thus, the true solution can be written as

\[
(3.8) \quad \xi^{(k)}(\theta_{i}) = u^{(k)}(\theta_{i}) + \sum_{r=k+1}^{\infty} \frac{\vartheta_{i}^{r+1}}{(r+1)!} D^{-k}(X \circ \xi).
\]
A comparison of (3.7) and (3.8) leads to the desired results.

Property 2 can be proved in a similar fashion, provided we start with

\[ \xi_i^{(k)} = u_i^{(k)}(1) + \sum_{j_1, k_0} \delta_{i k_0 j_1} \xi_j^{(k)}(1) - u_j^{(k)} + \sum_{j_2} a_{i j_2}(x^{(k)}(j_2) - R_{j_2}) \]

which will be true if Conditions A are satisfied. These conditions are explicitly stated below, but, in short, they are those conditions that arise by requiring that any \( \xi_i \) can be written as \( \xi_i = u(\theta_i) + \ldots \) which also are the same conditions that arise when we require that a scheme be exact for polynomials up to a certain order.

Thus, (3.5) defines a set of functions which contains the true solution \( \xi \) and the approximations \( \xi_i \). Hence, the problem of finding a CRK scheme can be stated as follows: Let \( \xi \) be the solution vector of (3.4). Let \( \xi_i(1) \) be defined by (3.5). Write the Taylor's expansions of \( \xi \) and \( \xi \) as

\[ \xi^{(k)}(\theta_i) = u^{(k)}(\theta_i) + \sum_{r=1}^{\infty} \frac{\theta_i}{(r+1+k)!} D^r(X \circ \xi)(0) \]

\[ \xi_i^{(k)}(1) = u_i^{(k)}(1) + \sum_{r=1}^{\infty} \frac{1}{(r+1+k)!} D^{r+1+k}(X \circ \xi_i)(0). \]

Choose the parameters \( g \) and \( f \) that appear in \( \xi \) so that these two series agree to a given order. When the parameters are chosen, Property 2 establishes the explicit representation of the scheme.

It is evident from (3.10) that we must calculate the derivatives of \( X \circ \xi \) and of \( \xi_i^{(k)} \). In what follows, we shall exhibit a set of functions into which these derivatives may be expanded. Property 1 suggests that it is only necessary to calculate the derivatives of \( \xi_i^{(k)} \) starting with \( D^{t+1} \xi_i^{(k)}(0) \).
More specifically

\[ \eta_1^{(k)}(0) = D^{r+1} \eta_1^{(k)}(0) = \frac{(r+1+k)!}{r!} D^{r} \eta_1^{(k)}(0) \]

for \( r \geq 1 \). We can, however, write

\[ \eta_1^{(k)} = \sum_{j, k_0} \eta_{j}^{(k_0)} + \sum_{j} [X \cdot u_j + \sum_{s} \frac{1}{s!} D_{L_1}^{(r)}...L_s^{(r)} X \cdot u_j n_{jL_1}...n_{jL_s}] \]

which, when the expansion of the second term is carried out, becomes

\[ \eta_1^{(k)} = \sum \eta_{j}^{(k_0)} + \sum [X \cdot u_j + \sum_{s} \frac{1}{s!} D_{L_1}^{(r)}...L_s^{(r)} X \cdot u_j n_{jL_1}...n_{jL_s}] \]

Differentiate \( \eta_1^{(k)} \), multiply both sides by \( \frac{(r+1+k)!}{r!} \), make use of the matrices \( i_{LN}^{(k)} \) and equation (3.11) to obtain

\[ D^{r+1+k} \eta_1^{(k)}(0) = \sum_{j} \frac{(r+1+k)!}{r!} f_{ijr}^{(k)} D^{r}(X \cdot u_j)(0) + \]

\[ \sum_{j} \sum_{s=1}^{\infty} \sum_{i_1,...,i_s,k_1,...,k_s} \frac{1}{s!} \alpha_{i_1...i_s}^{r+1+k} \]

\[ \sum_{j,k_0} \frac{(r+1+k)!}{r!} g_{ik_0j}^{(k)} D^{r-k_0+k_0} \eta_j^{(k_0)}(0) \]

where the extra value of \( k_1 \) has been deliberately displayed and

\[ \alpha_{i_1...i_s} = \binom{r}{i_1} \binom{i_1}{i_2} ... \binom{i_{s-1}}{i_s} \]
Since $D^r h_i^{(k)}(0) = 0$ for $r < \ell + 1 + k$, the range of the indices in (3.12) can be restricted to the following set which is referred to as the normal index set.

\begin{align*}
0 \leq k_j &\leq i_j - i_{j+1} - (\ell + 1), \quad j = 1, 2, \ldots, s-1 \\
0 \leq k_s &\leq i_s - (\ell + 1) \\
0 \leq k_o &\leq r - (\ell + 1) \\
(\ell + 1) \leq i_1 &\leq r \\
(s - j + 1)(\ell + 1) &\leq i_j \leq i_{j-1} - (\ell + 1), \quad j = 2, 3, \ldots, s \\
1 &\leq s \leq r \div (\ell + 1)
\end{align*}

(3.13)

where it is assumed that $k_i \in \bar{P} \subset P = \{0, \ldots, p - 1\}$ for all $k$, $\bar{P} = \{k \mid \xi^{(k)} \text{ explicitly appears in } X \circ \xi\}$, and $\div$ is used to denote an integer divide. Note that the upper bounds on $k$ will not be achieved if the upper bound is not in $\bar{P}$.

We also have the following bounds,

\begin{align*}
(\ell + 1) &\leq i_j - i_{j+1} \leq r + (1 - s)(\ell + 1), \quad j = 1, 2, \ldots, s - 1 \\
(\ell + 1) &\leq i_s \leq r + (1 - s)(\ell + 1)
\end{align*}

(3.14)

from which we can obtain

\begin{equation}
0 \leq k_i \leq r - s(\ell + 1), \quad i = 1, 2, \ldots, s.
\end{equation}

(3.15)

By convention, if $r \div (\ell + 1) = 0$, then the sum on $s$ is empty.

These bounds are explicitly displayed since it is necessary to have available the index bounds when determining whether we have obtained all the weighted differentials, derivative harmonics, etc., that we shall now proceed to define.
An examination of (3.12) shows that $D^{r+1+k} \eta_1^{(k)}(0)$, for any $k \in \mathbb{F}$, is expressed in terms of lower order derivatives. Therefore, if the lowest order derivative is known, the next derivative can be obtained and, thus, it is possible to obtain all derivatives.

Before defining functions $w^{(k)} \in R \rightarrow R^n$, called weighted differentials, that will allow us to expand the derivatives of $\eta_1^{(k)}$, we give a generic definition that helps simplify the presentation and, at the same time, illustrates that all derived quantities are obtained in, essentially, the same manner.

**Definition 3:**

The symbol $y_1^k$ is a generic $y$ of rank $R$, order $r$, degree $s = 0$, position 1, with $R = r$ if, and only if

$$y_1^k[R, r, 1] = Y_1^k[R] \circ (z_j^k[R - 1, r - 1, 0])$$

where $z_j^k$ is a generic $z$ of rank $R - 1$, order $r - 1$, position 0, degree 0. The symbol $y_1^k$ is a generic $y$ of rank $R$, order $r$, degree $s > 0$, position 1 if

$$y_1^k[R, r, a] = Y_1^k[R, k_0] \circ (z_j^{k_0}[R_0, r_0, a_0])$$

where $R = 1 + R_0 + k_0$, $r = r_0$, and $z_j^{k_0}$, is a generic $z$ of rank $R_0$, order $r_0$, degree $s$, position $a_0 \neq 0$, or if

$$y_1^k[R, r, a] = Y_1^k[R, r_0, k_1, \ldots, k_s] \circ (z_j^{k_1}[R_1, r_1, a_1], \ldots, z_j^{k_s}[R_s, r_s, a_s])$$

where
\[ R = 1 + r_0 + \sum_{j=1}^{s} (k_j + R_j) \]
\[ r = 1 + r_0 + \sum_{j=1}^{s} (k_j + r_j) \]

and \( z_j \) are generic \( z \) of rank \( R_i \), order \( r_i \), position \( a_i \) \( \neq 0 \). In all cases, \( Y \circ \) is the generic operator of the definition.

This definition is completed by requiring that Properties 1 - 4 stated below are true.

**Property 1**: A permutation of the elements of the set \( \{ k_i \} \) is equivalent to the same permutation of the elements of the set \( \{(R_i, r_i, a_i)\} = \{n_i\} \) and, in general, yields a new generic \( y \).

**Property 2**: A permutation of the elements of the set \( \{ k_i \} \) followed by an identical permutation of the elements of the set \( \{(R_i, r_i, a_i)\} = \{n_i\} \) does not yield a new generic \( y \). That is, any permutation of the set \( \{(k_i, R_i, r_i, a_i)\} = \{n_i\} \) yields the same generic \( y \).

**Property 3**: If \( k_i = k_j \), then the permutation of \( (R_i, r_i, a_i) \) with \( (R_j, r_j, a_j) \) does not yield a new \( y \). Likewise, if \( (R_i, r_i, a_i) \) is identical to \( (R_j, r_j, a_j) \), then the permutation of \( k_i \) with \( k_j \) does not yield a new \( y \).

**Property 4**: Given \( y \) defined by (3.18) of rank \( R \), order \( r \), degree \( s \), position \( a \), we obtain all distinct \( y \) with the same rank, order, and degree containing the same factors by considering all distinct permutations of \( (k_1, \ldots, k_s) \) with the understanding that if \( (R_i, r_i, a_i) = (R_j, r_j, a_j) \) then the permutation is not distinct. That is, associate to the couples \( (k_i, (R_i, r_i, a_i)) \) the integer \( n_i \). Two couples are considered equal if either \( k_i = k_j \) or \( (R_i, r_i, a_i) = (R_j, r_j, a_j) \) or both. Distinct couples have distinct integers \( n_i \). Form all the distinct permutations of the
set \( \{n_i\} \). Then, the correspondence \( n_i \rightarrow k_i \) or \( n_i \rightarrow (R_i, r_i, a_i) \) will furnish all the distinct \( y \) with the same factors.

Properties 3 and 4 are a consequence of Properties 1 and 2. It is necessary to adhere to these rules because in the generation of the quantities that follow, we must obtain all quantities, but we must also never repeat a quantity twice. A more detailed discussion is given in [5, p. 55].

If desired, a normal form can be obtained as \( y = Y \circ ((z_1)^{\mu_1} \cdots (z_\sigma)^{\mu_\sigma}) \) with \( s = \sum_{r=1}^{\sigma} \mu_i \) by means of suitable permutations and reindexing. In the above definition and subsequent realizations, it is always assumed that \( R \geq r \geq i + 1 \) and \( k_i \in \mathbb{P} \).

The weighted differentials \( W \) can be defined as follows:

Definition 4: Let

\[
Z_j^k \equiv \begin{cases} 1, & j = 1, \\ y_j^{k_i}[R_i, r_i, a_i] = y_j^{k_i}[R_i, r_i, a_i], & a_i \neq 0 \end{cases}
\]

\[
Y_1^k[R, r_0, k_0] = \sum_j \frac{(R+k)!}{(R-1)!} f_{ijR} C_{jN_0}^{(R)} 
\]

(3.19)

\[
Y_1^k[R, r_0, k_0, \ldots, k_s] = \sum_j \frac{(R+k)!}{(R-1)!} f_{ijR} C_{jN_0N_1 \ldots N_s}^{(R, k_1, \ldots, k_s)}
\]

where

\[
C_{jN_0N_1 \ldots N_s}^{(R, k_1, \ldots, k_s)} = D_{(D_{L_1} \cdots L_s X + u_j)^{N_0}} I_{L_1N_1 \cdots L_sN_s}^{(k_1) \cdots (k_s)}
\]

Then the generic \( y \) has as its realization the weighted differential \( W_1^k[R, r, a] \) of rank \( R \), order \( r \), position \( a \), degree \( s \).

After the fashion of Butcher [3], we use a shorthand notation and
write \((R-1)^{(k)}\) for (3.16), \(E^{(k)}(W^{(k_0)})\) for (3.17) and 
\(\langle r_0, k_1, \ldots, k_s; W_1, \ldots, W_s \rangle^{(k)} \) or 
\(\langle K; W_1^{(q)}, \ldots, W_s^{(q)} \rangle^{(k)}\) for (3.18) 
where \(K = (r_0, k_1, \ldots, k_s)\). Note that when using this abbreviated 
notation the subscript on \(W\) simply serves to indicate that these are 
different \(W\).

The actual generation (tabulation) of these quantities is given 
in \([5]\). To arrive at the results we wish to derive, it is not necessary 
to do that here. However, a few comments are in order about how one 
can think of these quantities. To obtain the \(y\), we start with the lowest 
\(R\) and \(r\), \(s = 0\), and work upward in order and in rank completing the sets 
with like order and rank as we proceed. It is convenient to envision the 
elements of constant order \(r\) and increasing rank \(R\) to form the rows and 
the elements of constant rank \(R\) and increasing order \(r\) to form the 
columns of a square array. The best way to become familiar with the 
structure of these elements is to carry out some examples. To show how 
this can be done, we give in Table I a short, incomplete, tabulation. 
It is immediately evident that we have assumed a 1 - 1 correspondence 
between \(y\) and \(z\), except for \(z^{[R-1,r-1,0]}\). This is not inherent in the 
definition, but since we shall have this correspondence in the examples 
given here, we assume that this is the situation.

In (3.19), the definition of the weighted differentials was explicitly 
written out. All the quantities used have almost an identical definition 
pattern. These quantities are all defined in Table II and definitions 
similar to Definition 4 can be arrived at by using this table.

The expansions of the derivatives of \(\eta_i^{(k)}\) are arrived at by means of
Theorem 1:

Let \( R \geq l + 1, k \in \mathbb{F}, S_R = \{ j \mid W_{ij}^{(k)}[R, r, j] \text{ has rank } R, \text{ order } r \} \). Let \( \alpha_{Rrj}^{(k)} \) be the derivative harmonic corresponding to the weighted differential \( W_{ij}^k [R, r, j] \). Then

\[
D^{R+k} \eta_{ij}^{(k)}(0) = \sum_{r=l+1}^{R} \sum_{j \in S_R} (R + k)! \alpha_{Rrj}^{(k)} W_{ij}^{(k)}[R, r, j](0).
\]

The derivative harmonics are non-negative, rational coefficients independent of \( i \) and are defined in Table II.

Proof: The proof is inductive. Assume (3.20) is true and consider the case \( R = l + 1 \). From (3.12), \( D^{l+1+k} \eta_{ij}^{(k)}(0) = 1 \cdot (l+1)^{(k)}(0) \) since \( l \div (l + 1) = 0 \). Now assume (3.20) true for all ranks less than \( R \) and substitute (3.20) into (3.12). It will be seen that the derivative harmonics furnish the correct coefficient for the degree zero terms and for the terms obtained using the \( E \) operator. The only question is the general coefficient of the second term in the right member of (3.12) after this substitution is carried out. To establish the validity of this term, write the expansion (3.20) for the left side of (3.12) and then establish the valid choices for the indices on the right side by permuting the couples \( (k_i, R_i, r_i, a_i) \) that appear as factors in the general term. The general coefficient that will be obtained will be the derivative harmonic \( \alpha_{Rrj}^{(k)} \) where we interpret \( a_i \) to be the number of times that \( (k_i, R_i, r_i, a_i) \) appears in its definition. A more detailed proof can be found in [5].

We now wish to use the differentials \( A \) and the weighted polynomials \( \phi \) as defined in Table II. An abbreviated brace notation is used for
the A and a bracket notation for the \( \Phi \). Thus, \((3.16), (3.17), \) and \((3.18)\) become \([r - 1], \mathcal{A}(A), \{r_0, k_1, \ldots, k_s; A_1, \ldots, A_s\}\) for the A and \([r - 1]^{(k)}, \mathcal{G}(k)(\Phi(k_0)), \{r_0, k_1, \ldots, k_s; \Phi_1, \ldots, \Phi_s\}\) for the \( \Phi \).

The expansion of the derivatives of \( X \circ \xi \) is accomplished using

**Theorem 2:**

\[
D_{-1}^r(X \circ \xi)(0) = \sum_{a \in S_r} \beta_{ra} A(r, a)(0)
\]

where \( \beta_{ra} = (r + k)! \alpha_{tra}^{(k)} \) for any \( k \in \mathbb{F} \) and \( S_r = \{a|A(r, a)\} \) has order \( r \).

**Proof:** The proof of these results follows directly from Theorem 1 when use is made of Property 1 of the \( \xi \) and it is noted that the choice of \( g \) and \( f \) causes the \( W \) to reduce to the differentials \( A \).

The weighted differentials \( W \) are factored using

**Theorem 3:**

\[
W_i^{(k)}[R, r, j] = \Phi_i^{(k)}[R, r, j] \cdot A(r, a)
\]

where \( W, \Phi, \) and \( A \) are as defined in Table II. More explicitly

\[
(r - 1)^{(k)} = [r - 1]^{(k)} \cdot \{r - 1\}
\]

\[
\mathcal{E}(k)((K; w(k_1), \ldots, w(k_s))) = \mathcal{G}(K; \Phi^{(k_1)}, \ldots, \Phi^{(k_s)}).
\]

\[
W_i^{(k)}[K; w(k_1), \ldots, w(k_s)] = [K; \Phi^{(k_1)}, \ldots, \Phi^{(k_s)}].
\]

\[
[K; A[r_1], \ldots, A[r_s]]\]

where \( K = (r_0, k_1, \ldots, k_s) \), the correspondence \( W_i^{(k_1)} = \Phi^{(k_1)}A[r_1] \) is assumed, \((k, k_1) \subseteq \mathbb{F}, \) and \( j \in S_R = \{j|W \text{ has rank } R, \text{ order } r\} \).

**Proof:** The proof is inductive using the definitions of \( W, \Phi, \) and \( A \).
The results are true for $s = 0$, $R = r$ so the process can be started. It can be shown that if they are true for degree $s$, order $r$, and rank $R$, then they are true for rank $R + 1$, and that they are also true for order $r + 1$.

The substitution of (3.20), (3.21), and (3.22) into (3.10) yields the following expansions for the solution $\xi$ and approximation $\zeta$.

$$
\xi(k)(\theta_1) = u(k)(\theta_1) + \sum_{r=1}^{\infty} \sum_{a \in S_r} \frac{\theta_1^{r+k}}{(r+k)!} A[r, a](0)
$$

$$
\zeta(k)(1) = u(k)(\theta_1) + \sum_{r=1}^{\infty} \sum_{a \in S_r} \left( \sum_{R=r}^{\infty} \sum_{j \in S_{Ra}} \alpha^{(k)}_{Rrj} \phi[j][R, r, j] \right) A[r, a](0)
$$

where $S_r = \{ a | A[r, a] \text{ has order } r \}$

$S_{Ra} = \{ j | W^{(k)}[R, r, j] \text{ has rank } R, \text{ order } r, \text{ and corresponds to } A[r, a] \text{ of order } r \}$

Equation (3.23) gives the desired expansion. However, it is possible to factor $\phi$ into a numerical coefficient $\gamma$ and an algebraic term $\Gamma$ allowing us to write $\alpha \gamma \Gamma$. It is also possible to collect the product $\alpha \gamma = \pi$ and write $\pi \Gamma$ where only two types of quantities appear in the summation; the numerical coefficient $\pi$ and the algebraic coefficient $\Gamma$. Finally, we can write $H = \alpha \phi$. The various representations have their advantages depending on what is of interest and how the results are to be obtained. These quantities are defined in Table II.

These various representations are obtained by using Theorem 1:

Let the generic $y$ of Definition 3 be generated as $y = Y z_1 \cdots z_s$
where \( Y = UV \) and \( z_i = u_i v_i \) are permissible factorizations of \( Y \) and \( z \).

Then \( y = y_1 y_2 \) is a permissible factorization of \( y \) where \( y_1 = u_1 \ldots u_s \) and \( y_2 = v_1 \ldots v_s \) are the generations of the factors \( y_1, y_2 \), provided the necessary commutations can be carried out. The converse is also true. That is, given the factors \( y_1 \) and \( y_2 \) generated using \( U \) and \( V \), then \( y = y_1 y_2 \) can be generated using the operator \( Y = UV \) provided the necessary cummutations can be carried out.

**Proof:** The proof is inductive starting with \( y[R, r, 1] \) of lowest rank, order, and degree.

This result allows us to write the coefficients of \( A \) in (3.23) as follows:

**Theorem 5:**

Let \( \alpha \) and \( \Phi \) be respectively a derivative harmonic and a weighted polynomial of rank \( R \), order \( r \), degree \( s \), position \( j \); then

\[
\alpha^{(k)}(k)_{R, r, j} = \alpha^{(k)}(k)_{R, r, j} \Gamma^{(k)}_{R, r, j} \]

(3.24)

where \( \gamma, \Gamma, \pi, \) and \( H \) are respectively the polynomial weights, elementary polynomials, product coefficients, generalized RK harmonics defined in Table II.

These results can be used to restate the generalized RK scheme in terms of the harmonics of the basis \( A \). To define a GRK scheme for the solution of (3.41), specify the rank \( q \), the extent \( e \), and the scheme
definition (3.6) with

\[ j_1 \in S_{j_1}, j_2 \in S_{j_2}, i \in S_i \]

where

\[ S_{j_1} \cup S_{j_2} \cup S_{j_2} \subset S = \{j | 0 \leq j \leq n \} \]

To determine the scheme parameters, choose an \( i \) in \( S \) and require that the corresponding \( \xi_i \) match the true solution \( \xi(\theta_i) \) to a certain order \( \bar{r} \).

This gives

\[
(3.25) \quad \sum_{R=r}^{\infty} \sum_{j \in S_{Ra}} R_i^{(k)}[R, r, j] - \beta_{Ra} \frac{\theta_i^{r+k}}{(r+k)!} = \xi(k)[R, a] = 0
\]

where

\[
l + 1 \leq r \leq \bar{r}
\]

\[ k \in P, a \in S_r = \{a | A[r, a] \text{has order } r \}
\]

\[ S_{Ra} = \{j | y_i^{(k)}[R, r, j] \text{ has rank } R, \text{ order } r, \text{ and corresponds to } A[r, a] \}.
\]

The conditions that the coefficients must satisfy when it is required that \( \xi_i^{(k)} - \xi(k)(\theta_i) = \mathcal{O}(h^{l+1+k}) \) be true for all \( i \in S_i \) are given as

**Conditions A:** Let \( \theta_i = \theta_i(t) \) and define the polynomials

\[
R_i^{(k)}(t) = \sum_{j_1} \frac{\theta_{j_1}^{l+k_0}}{(l+k_0)!} \sum_{k_0} \sum_{j_2} a_{j_2}^{(k)} \theta_{j_2}^{l-1} - \frac{\theta_i^{l+k}}{(l+k)!}.
\]

Then, in order that \( \xi_i^{(k)} - \xi(k)(\theta_i) = \mathcal{O}(h^{l+1+k}) \), it is necessary and sufficient that \( D^{R_i^{(k)}}(t) = 0 \) for \( r = 0, 1, \ldots, l + p - 1, k \in P, i \in S \).

If (3.25) and Conditions A are satisfied, then the local truncation
error is given by

\[ (3.26) \quad \xi_i^{(k)}(\theta_1) = \sum_{r,a} \varepsilon^{(k)}_{r,a} A[r, a] \]

where

\[ \overline{r} < r < \infty \]
\[ a \in S_r. \]

Equation (3.23) shows that any \( \xi_i \) can be written as a linear combination of the differentials \( A \). To be more explicit, we have

**Theorem 6:**

If \( \xi_i^{(k)} \) is an approximation defined by a CRK scheme, then

\[ (3.27) \quad \xi_i^{(k)} = u^{(k)}(\theta_1) + \sum_{r=\ell+1}^{\infty} \sum_{a \in S_r} \psi_{\ell a}^{(k)} A[r, a](0) \]

where the \( \psi \) are the approximation harmonics defined in Table II. This, in particular, includes the solution \( \xi(\theta_1) \).

**Proof:** Because of the validity of Conditions A, any approximation can be written as (3.9). If (3.27) is substituted into (3.9) an expansion is obtained in terms of \( A \). The isolation of the coefficients in the left and right numbers of the resultant expression will yield the approximation harmonics as given in Table II.

Since it is obvious that

\[ \psi_{\ell a}^{(k)} = \sum_{R=r}^{\infty} \sum_{J \in S_{Ra}} H_{\ell}^{(k)}[R, r, J], \]

the \( \psi \) can be used in (3.25) and the nonlinear parameter defining equations become

\[ \psi_{\ell a}^{(k)} = \beta_{\ell a}^{r+k} \frac{S_{\ell}^{r+k}}{(r+k)!}. \]
It is this form that is probably most useful when obtaining the parameter equations for a particular example.

We thus see that for GRK schemes, we can tabulate the equations that define the scheme parameters with no specific reference to the index sets and that the specialization to a particular scheme arises by specifying the index sets. This, then, gives a global view of the parameter equations that could prove useful in understanding their structure and, hence, helpful in solving the systems of equations. A short table of approximation harmonics is given in Table III.

We conclude this section with a few comments on the preceding development. It is interesting that by not specifying the accuracy of any approximation $\xi_i$, we are able to arrive at results that allow us to reduce the profusion of equations by always taking $l$ as large as possible. Butcher [3] took what would here be called the $l = 0$ case for Runge-Kutta methods. He could have taken $l = 1$, but for this particular case, the number of equations is the same. But, this is not true for cases where it is possible to take $l > 1$. Ceschino-Kuntzmann [4] have taken $l = 1$ and have split $\xi = u + v$ so their results are directly comparable for RK schemes and can serve as a check on these results.

It should be noted that the generic definition is always used to establish any particular quantity and that in order to insure obtaining the correct index sets, one should think of all quantities as being generated in parallel; any particular result being obtained by properly interpreting $y, z, Y$ at a particular set of indices. This is absolutely crucial in deriving these results.
When comparing truncation errors obtained by this means with those obtained from other derivations, it should be remembered that the differentials are made up out of various derivatives of $X \circ u$; whereas, most derivations use $X \circ \xi$. Thus, for example, neither our local error terms nor our equations are identical to those appearing in Butcher [1, 2].
IV. EXAMPLES

The examples presented here are meant to be only illustrative. The results derived in Section III are general and, in the author's view, will be best used to understand the structure of the parameter defining equations. That is, these results are global and will be best utilized in a global manner. A careful analysis of how the approximation harmonics are generated, how the various intermediate approximations enter into the final approximation, and the manner in which the parameters propagate; that is, how they are introduced usefully into the scheme, can possibly lead to the selection of schemes (starting, change of interval, integration), that are more accurate or more suitable for particular problems.

The obtaining of specific schemes depends on the tabulation of approximation harmonics; or, if desired, any of the equivalent harmonics. A short table is given in Table III. However, these quantities can all be obtained from Definition 3 of Section 3 and the definition itself can be represented as a suitably constructed algorithm that would then generate the harmonics.

Although, such an algorithm has not been built, the author has constructed an ALGOL 60 Program [5], along lines suggested by R. DeVogelaere [6], that arrives at the approximation harmonics by successively carrying out the required substitutions and linear combinations that define an approximation. The approach is based on results analogous to those developed here, but the view obtained is local; a particular scheme generates a particular set of equations. The global results presented here can, when used in conjunction with a constructive algorithm, provide not only an
overall view, but a parallel check of the results obtained from such a program.

However, to illustrate the actual use of the approximation harmonics, a general example is given below that contains many known schemes.

Consider the following problem:

**Problem 1.**

\[ \text{Dx} = X(x) \]

\[ x(\theta_q) = \xi_q \]

\[ \text{find } x(\theta_o) . \]

**Scheme 1**

\[ X_q = X(\xi_q) \]

\[ \text{for } i \in S_{q-1} \]

\[ \xi_i = \sum_{n \in S_{i_0}} a_{in} x_n + \sum_{n \in S_{i_1}} b_{in} X_n; X_i = X(\xi_i) \]

\[ \xi(\theta_o) = \xi_o + o(h^l) \]

where

\[ S_q = \{ q, q-1, \ldots, 0 \} \]

\[ S_{i_0} = \{ q, 2q, \ldots, kq \} \]

\[ S_{i_1} = S_{i_0} \cup (S_q - S_1) \]

and it is assumed that \( \theta_{(n-1)q} - \theta_{nq} = h \) for \( n = 1, 2, \ldots, k \).

Conditions A of Section III assure that all approximations are at least of order \( l \). This yields the following set of equations:

\[ \sum_{n \in S_{i_0}} a_{in} \frac{\theta_{n}}{j!} + \sum_{n \in S_{i_1}} b_{in} \frac{\theta_{n}^{j-1}}{(j-1)!} - \frac{\theta_{1}^{j}}{j!} = 0, j = 0, 1, \ldots, l \]

for \( i \in S_q \cup S_{i_0} \). Terms with a negative exponent are to be taken as
identically zero.

The approximation harmonics are given in Table IV where we can, for the purpose of determining the scheme parameters, take $\xi_i = \xi(\theta_i)$ when $i \in S_{10}$. The remaining parameter defining equations then become

\begin{equation}
\psi_{0j} = \beta_{0j}, \quad j = 0, 1, 2, \ldots .
\end{equation}

The extent to which (4.4) can be satisfied will determine $\alpha$ in (4.2).

In Table V are tabulated a number of examples that are contained in the scheme (4.2). It is interesting to note that all finite difference (FD) schemes are contained, $q = 1$ with arbitrary $k$. Also, all Runge-Kutta (RK) schemes, $k = 1$ with arbitrary $q$; however, for schemes of order higher than RK4, Table IV must be extended. Since most predictor-corrector (PC) schemes have a predictor and corrector that differ at most by one order, they can be considered as special applications of finite difference schemes. However, they are contained in (4.2) with $q = 2$, arbitrary $k$, and $\theta_0 - \theta_1 = 0$. Butcher's work is a generalization of these (PC) schemes and his off-step methods [1, 2] are also contained in (4.2).
V. COMMENTS

During the past few years, much interest has been displayed in generalized schemes for ordinary differential equations. It is believed that, most, if not all, of this work can be treated with the results derived in Section III. However, when $S_{10} = \{q, q+1, \ldots, kq\}$ it is necessary to have the harmonics of the off-step $i_1$, $i \in S_{10}$. This can be handled using undetermined parameters, and results for this have been developed [5]. The use of these results can become rather laborious and it seems better to proceed in a constructive fashion using, for example, the ALGOL 60 program that was previously mentioned and which can handle this case.

Also, schemes that use the first derivative DX after the fashion of Frey [7] are not contained here and the generalization of these results to those schemes does not seem to be obvious. These can, however, be handled in a constructive fashion using the above mentioned program.

Therefore, it would seem that the results developed here can best be used in better understanding the character of the parameter defining equations that arise from generalized (RK) schemes.
<table>
<thead>
<tr>
<th>Name</th>
<th>Definition</th>
<th>Name</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$y^k [R, r, 1]$</td>
<td>$y^k [R] \circ (z^k [R-1, r-1, 0])$</td>
<td>$y^k [R+1, r, 1]$</td>
<td>$y^k [R+1, 0] \circ (z^0 [R, r, 1])$</td>
</tr>
<tr>
<td>$y^k [R+1, r+1, 1]$</td>
<td>$y^k [R+1] \circ (z^k [R, r, 0])$</td>
<td>$y^k [R+2, r+1, 1]$</td>
<td>$y^k [R+2, 0] \circ (z^0 [R+1, r+1, 1])$</td>
</tr>
<tr>
<td>$y^k [R+1, r+1, 2]$</td>
<td>$y^k [R+1, 0, 0] \circ (z^0 [R, r, 1])$</td>
<td>$y^k [R+2, r+1, 2]$</td>
<td>$y^k [R+2, 0] \circ (z^0 [R+1, r+1, 2])$</td>
</tr>
<tr>
<td>$y^k [R+2, r+2, 1]$</td>
<td>$y^k [R+2] \circ (z^k [R+1, r+1, 0])$</td>
<td>$y^k [R+3, r+2, 1]$</td>
<td>$y^k [R+3, 0] \circ (z^0 [R+2, r+2, 1])$</td>
</tr>
<tr>
<td>$y^k [R+2, r+2, 2]$</td>
<td>$y^k [R+2, 1, 0] \circ (z^0 [R, r, 1])$</td>
<td>$y^k [R+3, r+2, 2]$</td>
<td>$y^k [R+3, 0] \circ (z^0 [R+2, r+2, 2])$</td>
</tr>
<tr>
<td>$y^k [R+2, r+2, 3]$</td>
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<td>$y^k [R+3, r+2, 3]$</td>
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</tr>
<tr>
<td>$y^k [R+2, r+2, 4]$</td>
<td>$y^k [R+2, 0, 0] \circ (z^0 [R+1, r+1, 2])$</td>
<td>$y^k [R+3, r+2, 4]$</td>
<td>$y^k [R+3, 0] \circ (z^0 [R+2, r+2, 4])$</td>
</tr>
<tr>
<td>$y^k [R+2, r+2, 5]$</td>
<td>$y^k [R+2, 0, 1] \circ (z^1 [R, r, 1])$</td>
<td>$y^k [R+3, r+2, 5]$</td>
<td>$y^k [R+3, 0] \circ (z^0 [R+2, r+2, 5])$</td>
</tr>
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<tr>
<td>$z^k_j[R-1,r-1,0]$</td>
<td>$y_j^k[R, r, a]$</td>
<td>$y_j^k[R, r, a]$</td>
<td>$y_j^k[R, r, a]$</td>
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<tr>
<td>$z^k_j[R, r, a]$</td>
<td>$y_j^k[R, r, a]$</td>
<td>$y_j^k[R, r, a]$</td>
<td>$y_j^k[R, r, a]$</td>
</tr>
<tr>
<td>$Y^k_1[R]$</td>
<td>$\frac{(R+k)!}{(R-1)!} \xi \theta^R R$</td>
<td>$\sum_{j} \frac{(R+k)!}{(R-1)!} \xi \theta^R R$</td>
<td>$\theta^R R$</td>
</tr>
<tr>
<td>$Y^k_1[R, k_o]$</td>
<td>$\frac{(R+k)!}{(R-1)!} \xi \theta^R R$</td>
<td>$\sum_{j} \frac{(R+k)!}{(R-1)!} \xi \theta^R R$</td>
<td>$\theta^R R$</td>
</tr>
<tr>
<td>$Y^k_1[R, r_0, k_1, \ldots k_s]$</td>
<td>$\frac{(R+k)!}{(R-1)!} \xi \theta^R R$</td>
<td>$\sum_{j} \frac{(R+k)!}{(R-1)!} \xi \theta^R R$</td>
<td>$\theta^R R$</td>
</tr>
<tr>
<td>$y_i^k[R, r, a]$</td>
<td>$w_i^k[R, r, a]$</td>
<td>$\Phi_i^k[R, r, a]$</td>
<td>$A[r, a]$, $R = r$</td>
</tr>
<tr>
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<td>Elementary Polynomials</td>
<td>Polynomial Weights</td>
<td>Derivative Harmonics</td>
</tr>
<tr>
<td>------------------</td>
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<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>( k_{j}[R, r, a] )</td>
<td>( k_{j}[R, r, a] )</td>
<td>( k_{j}[R, r, a] )</td>
</tr>
<tr>
<td>3</td>
<td>( \sum \frac{(k)}{j} \frac{r_{j}}{R} )</td>
<td>( \frac{(R + k)!}{(R - 1)!} )</td>
<td>( \frac{1}{(R + k)!} )</td>
</tr>
<tr>
<td>4</td>
<td>( \sum \frac{(k)}{j} \frac{g_{j}}{R} )</td>
<td>( \frac{(R + k)!}{(R - 1)!} )</td>
<td>( \frac{(R_{0} + k_{0})!}{(R + k)!} )</td>
</tr>
<tr>
<td>5</td>
<td>( \sum \frac{(k)}{j} \frac{r_{o}}{R} )</td>
<td>( \frac{(R + k)!}{(R - 1)!} )</td>
<td>( \frac{(R-1)!}{(R+k)!} \frac{1}{r_{o}(\omega_{1})!...\omega_{o})!} )</td>
</tr>
</tbody>
</table>

where \( \omega_{1} \) is the number of times that \( (k_{1},r_{1},a_{1}) \) appears as a factor in \( y_{j}[R, r, a] \).

where \( \omega_{1} \) is as defined for the derivative harmonics.
TABLE II. Cont'd.

<table>
<thead>
<tr>
<th>Generalized FK Harmonics</th>
<th>Approximation Harmonics</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k_{0} = (k_{1} + R + k_{2}, r, a)_{R = r; 0 &lt; R}$</td>
<td>$k_{0} = (k_{1} + R + k_{2}, r, a)_{R = r; 0 &lt; R}$</td>
</tr>
</tbody>
</table>

Note: $\psi_{k_{0}} = z_{k_{0}}$ is defined in terms of $z$ and not $y$. Where $\psi_{k_{0}}$ are as defined for derivative harmonics.
### TABLE III

**APPROXIMATION HARMONICS** $\psi$

<table>
<thead>
<tr>
<th>$k \varepsilon P C P = {0, \ldots, p-1}$</th>
<th>$k \varepsilon P C P = {0, \ldots, p-1}$</th>
<th>$k \varepsilon P C P = {0, \ldots, p-1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\psi$</td>
<td>$\psi$</td>
<td>$\psi$</td>
</tr>
<tr>
<td>$0$</td>
<td>$0$</td>
<td>$0$</td>
</tr>
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<td>$20$</td>
</tr>
<tr>
<td>$15$</td>
<td>$21$</td>
<td>$21$</td>
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</tbody>
</table>

\[
q^k \psi = \sum_{i=0}^{p-1} f_{i}^k e^{i \phi} \psi_{i}^k \\
F \phi = \sum_{\alpha=1}^{p} \frac{f_{\alpha}^k}{\alpha!} \psi_{\alpha}^k \\
F \psi_{\alpha_1} \psi_{\alpha_2} = \sum_{\alpha=1}^{p} \frac{f_{\alpha}^k}{\alpha!} \psi_{\alpha_1} \psi_{\alpha_2} \\
F^k \psi_{\alpha_1} \psi_{\alpha_2} = \sum_{\alpha=1}^{p} \frac{f_{\alpha}^k}{\alpha!} \psi_{\alpha_1} \psi_{\alpha_2}
\]
### TABLE IV
APPROXIMATION HARMONICS FOR SCHEME 1

<table>
<thead>
<tr>
<th>( i(\theta_i) )</th>
<th>( \Sigma_{n \in S_{10}} a_{in} \psi_{no} + \Sigma_{n \in S_{11}} b_{in} \theta_n / l! )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( j )</td>
<td>( \psi_{ij} = \beta_{ij} )</td>
</tr>
<tr>
<td>( \psi_{ij} )</td>
<td></td>
</tr>
<tr>
<td>( h^1 )</td>
<td>0 ( \theta_1^1 / (l+1)! )</td>
</tr>
<tr>
<td>( \Sigma_{n \in S_{10}} a_{in} \psi_{no} + \Sigma_{n \in S_{11}} b_{in} \theta_n / l! )</td>
<td></td>
</tr>
<tr>
<td>( h^2 )</td>
<td>1 ( \theta_1^2 / (l+2)! )</td>
</tr>
<tr>
<td>( \Sigma_{n \in S_{10}} a_{in} \psi_{n1} + \Sigma_{n \in S_{11}} b_{in} \theta_n / (l+1)! )</td>
<td></td>
</tr>
<tr>
<td>( h^3 )</td>
<td>2 ( \theta_1^3 / (l+2)! )</td>
</tr>
<tr>
<td>( \Sigma_{n \in S_{10}} a_{in} \psi_{n2} + \Sigma_{n \in S_{11}} b_{in} \psi_{no} )</td>
<td></td>
</tr>
<tr>
<td>( h^4 )</td>
<td>3 ( \theta_1^4 / (l+3)! )</td>
</tr>
<tr>
<td>( \Sigma_{n \in S_{10}} a_{in} \psi_{n3} + \Sigma_{n \in S_{11}} b_{in} \theta_n / (l+2)! )</td>
<td></td>
</tr>
<tr>
<td>( h^5 )</td>
<td>4 ( (l+2) \theta_1^{l+3} / (l+3)! )</td>
</tr>
<tr>
<td>( \Sigma_{n \in S_{10}} a_{in} \psi_{n4} + \Sigma_{n \in S_{11}} b_{in} \psi_{n1} )</td>
<td></td>
</tr>
<tr>
<td>( h^6 )</td>
<td>5 ( \theta_1^{l+3} / (l+3)! )</td>
</tr>
<tr>
<td>( \Sigma_{n \in S_{10}} a_{in} \psi_{n5} + \Sigma_{n \in S_{11}} b_{in} \psi_{n1} )</td>
<td></td>
</tr>
<tr>
<td>( h^7 )</td>
<td>6 ( \theta_1^{l+3} / (l+3)! )</td>
</tr>
<tr>
<td>( \Sigma_{n \in S_{10}} a_{in} \psi_{n6} + \Sigma_{n \in S_{11}} b_{in} \psi_{n2} )</td>
<td></td>
</tr>
</tbody>
</table>
### TABLE V

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Reference</th>
<th>q</th>
<th>k</th>
<th>l</th>
<th>α</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>RK</td>
<td>[4]</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>Enter.</td>
</tr>
<tr>
<td>RK2</td>
<td>[4]</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>$\theta_1$ is a free parameter.</td>
</tr>
<tr>
<td>RK3</td>
<td>[4]</td>
<td>3</td>
<td>1</td>
<td>1</td>
<td>3</td>
<td>$\theta_1$, $\theta_2$ are free parameters.</td>
</tr>
<tr>
<td>RK4</td>
<td>[4]</td>
<td>4</td>
<td>1</td>
<td>1</td>
<td>4</td>
<td>$\theta_0 - \theta_1 = 0$, $\theta_2$, $\theta_3$ are free parameters.</td>
</tr>
<tr>
<td>Butcher</td>
<td>[1]</td>
<td>3</td>
<td>k</td>
<td>$2k - 1$</td>
<td>3</td>
<td>Stable, $\theta_2$ is a free parameter, $\theta_0 - \theta_1 = 0$.</td>
</tr>
<tr>
<td>Butcher</td>
<td>[2]</td>
<td>4</td>
<td>k</td>
<td>$2k - 1$</td>
<td>4</td>
<td>Stable, $\theta_2$, $\theta_3$ are free parameters, $\theta_0 - \theta_1 = 0$.</td>
</tr>
<tr>
<td>FD</td>
<td>[4]</td>
<td>1</td>
<td>k</td>
<td>$2k - 1$</td>
<td>1</td>
<td>Stability limits the use of all parameters.</td>
</tr>
<tr>
<td>PC</td>
<td>[4]</td>
<td>2</td>
<td>k</td>
<td>$2k - 1$</td>
<td>2</td>
<td>Stability limits the use of all parameters.</td>
</tr>
</tbody>
</table>
REFERENCES


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