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Error Estimation for Runge-Kutta Methods Through Pseudo-iterative Formulas. (**)

1. - Introduction.

Concerning RUNGE-KUTTA formulas for the numerical solution of differential equations $y' = f(x, y)$ it is objected that the process does not contain in itself any simple means for estimating the committed errors or detecting arithmetical mistakes [5]. This objection appears to be universally accepted, but is unfounded. In fact we shall put into evidence an error estimating internal property of RUNGE-KUTTA formulas irrespective of their order. This property is easy to apply, but weak, and will be improved with the derivation of families of new RUNGE-KUTTA type formulas of fifth order which will be said to have pseudo-iterative form [6]. In other articles pseudo-iterative formulas of order $n \geqslant 6$ will be treated [7].

The error estimates provided by the pseudo-iterative formulas of a given order compare favorably with those obtained from the presently known methods. In addition, pseudo-iterative formulas offer a more practical way and do not require any additional labor except that of performing a linear combination of a few k's already computed.

However, in all fairness it must be pointed out that all these methods gradually diminish in effectiveness as we progress step by step and that we are as yet far from possessing a satisfactory rigorous method for error estimation [2].

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2. – We are given the differential equation

$$\frac{dy}{dx} = f(x,\ y) \tag{1}$$

subject to the initial condition $x = x_0$, $y = y_0$. Let $y(x)$ be the solution of this initial value problem and let $\tilde{y}(x_0 + h)$ be an approximation to $y(x_0 + h)$, where h is the considered step-length.

It is known that RUNGE-KUTTA type formulas are defined as follows:

$$\tilde{y}_m(x_0 + h) = y_0 + \sum_{i=0}^{p} w_i\, k_i\,, \tag{2 a}$$

where m, $m \geqq p + 1$, is the order of the process and

$$\begin{cases} k_0 = h\, f(x_0\,, \quad y_0) \\ k_1 = h\, f(x_0 + a_1 h, \quad y_0 + a_1 k_0) \\ k_n = h\, f(x_0 + a_n h, \quad y_0 + \sum_{i=0}^{n-1} b_{n,i}\, k_i) \qquad (n = 2, \ldots, p) \end{cases} \tag{2 b}$$

with

$$a_n = \sum_{i=0}^{n-1} b_{n,i}\,.$$

We remark that at the first and second stage of (2 b) we can evaluate

$$\tilde{y}_1(x_0 + h) = y_0 + k_0 \tag{3}$$

and

$$\tilde{y}_2(x_0 + h) = y_0 + \left(1 - \frac{1}{2a_1}\right) k_0 + \frac{1}{2a_1}\, k_1\,, \tag{4}$$

which represent first and second order approximations to the true value $y(x_0 + h)$, respectively.

A comparison between the successively improved approximations $\tilde{y}_1(x_0 + h)$, $\tilde{y}_2(x_0 + h)$ and $\tilde{y}_m(x_0 + h)$, $m \geqslant 3$, will not only permit the detection of gross errors and arithmetical mistakes if any, but it will provide also some valuable information concerning the accuracy of the final result, $\tilde{y}_m(x_0 + h)$.

Let $e(x_0\,, y_0;\, n;\, h)$ represent the error in $\tilde{y}_n(x_0 + h)$. Then

$$y(x_0 + h) - \tilde{y}_2(x_0 + h) = e(x_0\,,\ y_0;\ 2;\ h)\,.$$

In general $\tilde{y}_m(x_0 + h)$, $m \geqslant 3$, is a far better approximation to the exact value $y(x_0 + h)$ than $\tilde{y}_2(x_0 + h)$. Thus according to accepted usage ([2], p. 52) replacing in the preceding equation $y(x_0 + h)$ by $y_m(x_0 + h)$ we have

$$\tilde{y}_m(x_0 + h) - \tilde{y}_2(x_0 + h) = e(x_0\,,\ y_0;\ 2;\ h)$$

or more appropriately

$$\tilde{e}(x_0\,,\ y_0;\ 2;\ h) = \tilde{y}_m(x_0 + h) - \tilde{y}_2(x_0 + h)\,,$$

where $\tilde{e}(x_0\,,\ y_0;\ 2;\ h)$ stands for an approximation to $e(x_0\,,\ y_0;\ 2;\ h)$.

Thus if $\tilde{e}(x_0, y_0;\ 2;\ h) \leqslant 5 \cdot 10^{-p}$ then we shall accept $\tilde{y}_2(x_0 + h)$ as an approximation for $y(x_0 + h)$ correct to p-decimal places and a fortiori $\tilde{y}_m(x_0 + h)$ to be an approximation correct at least to p-decimal places.

In other words the approximate values $\tilde{y}_m(x_0 + h)$ and $\tilde{y}_2(x_0 + h)$ are accepted to agree with the exact value $y(x_0 + h)$ about to the same accuracy as to which they agree with each other.

With the purpose of strengthening this method of attack to the error estimation problem we tried to imbed in a fourth order RUNGE-KUTTA formula a third order one. In this manner it was hoped that we would be able to compare a third order approximation with a fourth order one and thus obtain better error estimates. However, we have found that such a fourth order RUNGE-KUTTA formula does not exist, for it can be easily shown that the simultaneous presence of $\tilde{y}_3(x_0 + h)$ and $\tilde{y}_4(x_0 + h)$ is impossible in any one formula of order $n \geqq 4$.

After this negative result the investigation of an even more interesting problem that of the imbedment of a fourth order formula into a fifth order one, follows naturally and logically. Fortunately as it will be shown in subsequent paragraphs, this imbedment is possible. We may give as an example the formula:

$$\tilde{y}_5(x_0 + h) = y_0 + \frac{1}{336}(14k_0 + 35k_3 + 162k_4 + 125k_5)\,,$$

$$\begin{cases} k_0 = h\,f(x_0\,,\ y_0), & \tilde{y}_1(x_0 + h) = y_0 + k_0 \\ k_1 = h\,f\left(x_0 + \frac{1}{2}h,\ y_0 + \frac{1}{2}k_0\right), & \tilde{y}_2(x_0 + h) = y_0 + k_1 \\ k_2 = h\,f\left(x_0 + \frac{1}{2}h,\ y_0 + \frac{1}{4}(k_0 + k_1)\right) & \\ k_3 = h\,f(x_0 + h,\ y_0 - k_1 + 2k_2)\,, & \tilde{y}_4(x_0 + h) = y_0 + \frac{1}{6}(k_0 + 4k_2 + k_3) \\ k_4 = h\,f\left(x_0 + \frac{2}{3}h,\ y_0 + \frac{1}{27}(7k_0 + 10k_1 + k_3)\right) & \\ k_5 = h\,f\left(x_0 + \frac{2}{10}h,\ y_0 + \frac{1}{625}(28k_0 - 125k_1 + 546k_2 + 54k_3 - 378k_4)\right). & \end{cases}$$

Indeed at the fourth and sixth stage of this formula one can obtain by linear combination of appropriate k's, fourth and fifth order approximations to $y(x_0 + h)$, respectively. Besides this, as already mentioned, at its first and second stages it provides first and second order approximations.

This formula and the related error estimating internal property are readily extended to systems of first order differential equations. Indirectly but with equal ease they are extended also to differential equations of order $n \geqq 2$.

Let us show with a concrete example the effectiveness of this method and the ease with which it can be applied even in the case of higher order differential equations.

Consider the second order differential equation $(1 - x^2)y'' - 2\,x\,y' + 6\,y = 0$, subject to the initial conditions $x = 0$, $y = -\frac{1}{2}$, $y' = 0$. This being a LEGENDRE equation it has as solution the polynomial $y(x) = (3x^2 - 1)/2$. We find also $y'(x) = 3\,x$. Thus for a chosen step-size h the latter two functions permit the evaluation of the exact values $y(x_0 + h)$ and $y'(x_0 + h)$.

Through the use of the above fifth order formula (in its extended form) we find (with $h = 0.0125$):

$$\begin{cases} \tilde{y}_4 = -0.499\,765\,625\,003\,\underline{579\,9} \\ \tilde{y}_5 = -0.499\,765\,625\,000\,\underline{388\,0}, \end{cases} \qquad \begin{cases} \tilde{y}'_4 = 0.037\,499\,999\,\underline{791\,\,561\,13} \\ \tilde{y}'_5 = 0.037\,499\,999\,\underline{379\,118\,27}\,. \end{cases}$$

One can see in a glance that $\tilde{y}_4$ and $\tilde{y}_5$ have their leading 11 decimal figures in agreement. Then our method indicates that each of these values and particularly $\tilde{y}_5$ have also 11 leading decimal figures in agreement with the exact value.

Indeed this conclusion is true for $y = -0.499\,765\,625\,000\,000\,0$. We thus can write $\tilde{y}_5 = -0.499\,765\,625\,00$ and say that this approximation is correct to 11 decimal figures.

On the other hand $\tilde{y}'_4$ and $\tilde{y}'_5$ have only nine leading decimal figures in agreement. The exact value of y' is 0.0375 or $0.037\,499\,999\,\ldots$ which shows that truly these two approximate values are in nine decimal figure agreement with the exact value also.

If these approximate values are too accurate or not accurate enough according to given requirements, one may reduce or increase the accuracy of approximations simply by increasing or decreasing the step-size h. We shall not enter into more details at present. These are left to later sections.

Now that we have indicated the feasibility of imbedment of a fourth order RUNGE-KUTTA formula into a fifth order one and have provided an example of such a formula, we can give a specific definition to pseudo-iterative formulas.

Definition. Let $\{k_j\}$ $(j = 0, \ldots, q;\ q \geqslant 6)$ be the set of incremental coefficients associated with a certain RUNGE-KUTTA formula of order n

($5 \leqslant n \leqslant q$). This formula will be called a pseudo-iterative formula of order n if with a subset $\{k_i\}$ of $\{k_j\}$ ($i = 0, \ldots, p$; $p < q$) we can obtain a formula of order $n-1$, both formulas being valid at $x = x_0 + h$.

Then the above described method can be stated as follows:

Rule. If the approximate values $\tilde{y}_n(x_0 + h)$ and $\tilde{y}_{n-1}(x_0 + h)$ have their j leading decimal figures in agreement, then $\tilde{y}_n(x_0 + h)$ is in j decimal figure agreement with the exact value $y(x_0 + h)$.

A more rigorous proof or justification of this rule will be given in a subsequent article.

3. – It is well known that six substitutions or stages are necessary for the derivation of fifth order RUNGE-KUTTA formulas.

Thus, since $p = 5$, the relations (2 a), (2 b) may be written

$$\tilde{y}_5(x_0 + h) = y_0 + \sum_{i=0}^{5} w_i\, k_i\,, \tag{5 a}$$

where

$$\left\{\begin{aligned} k_0 &= h\, f(x_0\,,\ y_0) \\ k_1 &= h\, f(x_0 + a_1 h,\ y_0 + a_1 k_0) \\ k_2 &= h\, f(x_0 + a_2 h,\ y_0 + b_{2,1} k_1 + b_{2,0} k_0) \\ k_3 &= h\, f(x_0 + a_3 h,\ y_0 + b_{3,2} k_2 + b_{3,1} k_1 + b_{3,0} k_0) \\ k_4 &= h\, f(x_0 + a_4 h,\ y_0 + \sum_{i=0}^{3} b_{4,i} k_i) \\ k_5 &= h\, f(x_0 + a_5 h,\ y_0 + \sum_{i=0}^{4} b_{5,i} k_i) \end{aligned}\right. \tag{5 b}$$

with

$$a_n = \sum_{i=0}^{n-1} b_{n,i} \qquad (n = 2, \ldots, 5).$$

Then the usual matching procedure between the two truncated power series representing $y(x_0 + h)$ and $\tilde{y}_5(x_0 + h)$, as defined in (2 a) with $p = 5$, gives the following known system of 16 algebraic equations in 21 parameters:

$$\sum_{i=0}^{5} w_i = 1\,, \tag{I}$$

$$\sum_{i=1}^{5} w_i\, a_i^j = \frac{1}{j+1} \qquad (j = 1,\ 2,\ 3,\ 4)\,, \tag{II-V}$$

(VI-VIII) $$\sum_{i=2}^{5} w_i \sum_{j=1}^{i-1} a_j^n b_{i,j} = \frac{1}{(n+1)(n+2)} \qquad (n = 1,\ 2,\ 3),$$

(IX-X) $$\sum_{i=2}^{5} w_i\, a_i \sum_{j=1}^{i-1} a_j^n b_{i,j} = \frac{1}{(1+n)(3+n)} \qquad (n = 1,\ 2),$$

(XI) $$\sum_{i=2}^{5} w_i\, a_i^2 \sum_{j=1}^{i-1} a_j\, b_{i,j} = \frac{1}{10},$$

(XII) $$\sum_{i=2}^{5} w_i \left(\sum_{j=1}^{i-1} a_j\, b_{i,j}\right)^2 = \frac{1}{20},$$

(XIII-XIV) $$\sum_{i=3}^{5} w_i \sum_{j=3}^{i} b_{i,j-1} \sum_{m=1}^{j-2} a_m^n\, b_{j-1,m} = \frac{1}{12(1+n^2)} \qquad (n = 1,\ 2),$$

(XV) $$\sum_{i=3}^{5} w_i \sum_{j=1}^{i-2} b_{i,j+1}\,(a_{j+1} + a_i) \sum_{m=1}^{j} a_m\, b_{j+1,m} = \frac{7}{120},$$

(XVI) $$\sum_{i=4}^{5} w_i \sum_{j=3}^{i-1} b_{i,j} \sum_{m=2}^{j-1} b_{j,m} \sum_{n=1}^{m-1} a_n\, b_{m,n} = \frac{1}{120}.$$

Consider the set of incremental coefficients constituted by the first four stages of (5 b). In this set we let

(6) $$a_1 = a_2 = \frac{1}{2}, \quad a_3 = 1, \quad b_{2,1} = \frac{1}{2t}, \quad b_{3,1} = 1 - t, \quad b_{3,2} = t \neq 0,$$

where t is a free parameter. Then at the fourth stage of (5 b) the use of the formula

$$\tilde{y}_4(x_0 + h) = y_0 + \frac{1}{6}[k_0 + 4(2-t)\,k_1 + 2t\,k_2 + k_3]$$

will give as it is well known [4] a fourth order approximation to $y(x_0 + h)$.

In view of this we assign to the parameters a_i $(i = 1, 2, 3)$, $b_{2,1}$ and $b_{3,i}$ $(i = 1, 2)$, of the system of algebraic equations (I-XVI), the values as indicated in (6). We thus obtain the following new system:

(7.1) $$w_0 + w_1 + w_2 + w_3 + w_4 + w_5 = 1,$$

(7.2) $$\frac{1}{2}(w_1 + w_2) + w_3 + w_4\, a_4 + w_5\, a_5 = \frac{1}{2}$$

(7.3) $$\frac{1}{4}(w_1 + w_2) + w_3 + w_4\, a_4^2 + w_5\, a_5^2 = \frac{1}{3}$$

(7.4) $$\frac{1}{8}(w_1 + w_2) + w_3 + w_4\, a_4^3 + w_5\, a_5^3 = \frac{1}{4}$$

(7.5) $$\frac{1}{16}(w_1 + w_2) + w_3 + w_4\, a_4^4 + w_5\, a_5^4 = \frac{1}{5},$$

$$\left\{\begin{aligned}
&(7.6)\quad \frac{1}{2}\left[\frac{1}{2t}w_2 + w_3 + w_4(b_{4,1}+b_{4,2}) + w_5(b_{5,1}+b_{5,2})\right] + \\
&\qquad + (w_4 b_{4,3} + w_5 b_{5,3}) + w_5 a_4 b_{5,4} = \frac{1}{6} \\
&(7.7)\quad \frac{1}{4}\left[\frac{1}{2t}w_2 + w_3 + w_4(b_{4,1}+b_{4,2}) + w_5(b_{5,1}+b_{5,2})\right] + \\
&\qquad + w_4 b_{4,3} + w_5 b_{5,3}) + w_5 a_4^2 b_{5,4} = \frac{1}{12} \\
&(7.8)\quad \frac{1}{8}\left[\frac{1}{2t}w_2 + w_3 + w_4(b_{4,1}+b_{4,2}) + w_5(b_{5,1}+b_{5,2})\right] + \\
&\qquad + (w_4 b_{4,3} + w_5 b_{5,3}) + w_5 a_4^3 b_{5,4} = \frac{1}{20},
\end{aligned}\right.$$

$$\left\{\begin{aligned}
&(7.9)\quad \frac{1}{8t}w_2 + \frac{1}{2}\left[w_3 + w_4 a_4(b_{4,1}+b_{4,2}) + w_5 a_5(b_{5,1}+b_{5,2})\right] + \\
&\qquad + w_4 a_4 b_{4,3} + w_5 a_5(b_{5,3} + a_4 b_{5,4}) = \frac{1}{8} \\
&(7.10)\quad \frac{1}{16t}w_2 + \frac{1}{4}\left[w_3 + w_4 a_4(b_{4,1}+b_{4,2}) + w_5 a_5(b_{5,1}+b_{5,2})\right] + \\
&\qquad + w_4 a_4 b_{4,3} + w_5 a_5(b_{5,3} + a_4^2 b_{5,4}) = \frac{1}{15},
\end{aligned}\right.$$

$$(7.11)\quad \frac{1}{16t}w_2 + \frac{1}{2}\left[w_3 + w_4 a_4^2(b_{4,1}+b_{4,2}) + w_5 a_5^2(b_{5,1}+b_{5,2})\right] + $$
$$+ w_4 a_4^2 b_{4,3} + w_5 a_5^2(b_{5,3} + a_4 b_{5,4}) = \frac{1}{10},$$

$$(7.12)\quad \frac{1}{16t^2}w_2 + \frac{1}{4}w_3 + w_4\left[\frac{1}{2}(b_{4,1}+b_{4,2}) + b_{4,3}\right]^2 + $$
$$+ w_5\left[\frac{1}{2}(b_{5,1}+b_{5,2}) + (b_{5,3} + a_4 b_{5,4})\right]^2 = \frac{1}{20},$$

$$(7.13)\quad \frac{1}{2}\left\{\frac{1}{2}w_3 + w_4\left(\frac{1}{2t}b_{4,2} + b_{4,3}\right) + w_5\left[\frac{1}{2t}b_{5,2} + b_{5,3} + (b_{4,1}+b_{4,2})b_{5,4}\right]\right\} + $$
$$+ w_5 b_{4,3} b_{5,4} = \frac{1}{24},$$

$$(7.14)\quad \frac{1}{4}\left\{\frac{1}{2}w_3 + w_4\left(\frac{1}{2t}b_{4,2} + b_{4,3}\right) + w_5\left[\frac{1}{2t}b_{5,2} + b_{5,3} + (b_{4,1}+b_{4,2})b_{5,4}\right]\right\} + $$
$$+ w_5 b_{4,3} b_{5,4} = \frac{1}{60},$$

$$(7.15)\quad \frac{3}{8}w_3+\frac{1}{2}w_4\left[\frac{1}{2t}\left(\frac{1}{2}+a_4\right)b_{4,2}+(1+a_4)\,b_{4,3}\right]+$$
$$+\frac{1}{2}w_5\left[\frac{1}{2\,t}\left(\frac{1}{2}+a_5\right)b_{5,2}+(1+a_5)\,b_{5,3}+\right.$$
$$\left.+(a_4+a_5)\,(b_{4,1}+b_{4,2}+2b_{4,3})\,b_{5,4}\right]=\frac{7}{120}\,,$$

$$(7.16)\quad \frac{1}{4}w_4\,b_{4,3}+\frac{1}{2}w_5\left[\frac{1}{2}\,b_{5,3}+\left(\frac{1}{2\,t}\,b_{4,2}+b_{4,3}\right)b_{5,4}\right]=\frac{1}{120}$$

or better

$$\frac{1}{2}w_4\,b_{4,3}+w_5\left[\frac{1}{2}\,b_{5,4}+\left(\frac{1}{2\,t}\,b_{4,2}+b_{4,3}\right)b_{5,4}\right]=\frac{1}{60}\,.$$

This complex system of 16 algebraic equations is in 16 unknowns. Thus it appears to be a tight case. It will be shown however, that this is not so, for two of these equations will be discarded as dependent. This will leave 14 independent equations in 16 unknowns. Two of the latter, namely a_4 and a_5, will be taken as free parameters and the remaining 14 unknowns will be expressed in terms of them.

Consider the system of four equations (7.2)-(7.5). This system is linear in the unkonowns (w_1+w_2), w_3, w_4 and w_5. Let D represent the determinant of the coefficients, that is:

$$D=\begin{vmatrix}\frac{1}{2} & 1 & a_4 & a_5\\ \frac{1}{4} & 1 & a_4^2 & a_5^2\\ \frac{1}{8} & 1 & a_4^3 & a_5^3\\ \frac{1}{16} & 1 & a_4^4 & a_5^4\end{vmatrix}=\frac{1}{2}\,a_4\,a_5\begin{vmatrix}1 & 1 & 1 & 1\\ \frac{1}{2} & 1 & a_4 & a_5\\ \frac{1}{4} & 1 & a_4^2 & a_5^2\\ \frac{1}{8} & 1 & a_4^3 & a_5^3\end{vmatrix}.$$

The last one being a VANDERMONDE determinant, we find readily:

$$D=\frac{1}{4}\,a_4\,a_5\,(a_5-a_4)\,(a_5-1)\left(a_5-\frac{1}{2}\right)(a_4-1)\left(a_4-\frac{1}{2}\right).$$

With the assumption that $D\neq 0$, that is, with

$$(8)\qquad a_4\neq 0,\quad a_5\neq 0,\quad a_4\neq\frac{1}{2},\quad a_4\neq 1,\quad a_5\neq\frac{1}{2},\quad a_5\neq 1,\quad a_4\neq a_5,$$

the application of CRAMER's rule to the system (7.2)-(7.5), yields:

$$w_1 + w_2 = \frac{4[10\, a_4\, a_5 - 5(a_4 + a_5) + 3]}{15(2a_4 - 1)(2a_5 - 1)}, \tag{9.2}$$

$$w_3 = \frac{10\, a_4\, a_5 - 10(a_4 + a_5) + 9}{60(a_4 - 1)(a_5 - 1)}, \tag{9.3}$$

$$w_4 = \frac{1}{60\, a_4(a_5 - a_4)(2a_4 - 1)(a_4 - 1)}, \tag{9.4}$$

$$w_5 = \frac{-1}{60\, a_5(a_5 - a_4)(2a_5 - 1)(a_5 - 1)}. \tag{9.5}$$

Again the application of CRAMER's rule to the system of equations (7.6)-(7.8) yields:

$$\frac{1}{2t} w_2 + w_3 + w_4\,(b_{4,1} + b_{4,2}) + w_5\,(b_{5,1} + b_{5,2}) = \frac{2(5a_4 - 2)}{15(2a_4 - 1)}, \tag{9.6}$$

$$w_4\, b_{4,3} + w_5\, b_{5,3} = \frac{1}{60(1 - a_4)}, \tag{9.7}$$

$$w_5\, b_{5,4} = \frac{1}{60\, a_4(a_4 - 1)(2a_4 - 1)}. \tag{9.8}$$

The combination of (9.5) and (9.8) gives:

$$b_{5,4} = -\frac{a_5(a_5 - a_4)(a_5 - 1)(2a_5 - 1)}{a_4(a_4 - 1)(2a_4 - 1)}. \tag{9.8'}$$

Multiplying both sides of (7.10) by two and subtracting (7.9) from it we obtain:

$$w_4\, a_4\, b_{4,3} + w_5\, a_5\, b_{5,3} + w_5\, a_4\, a_5\,(2a_4 - 1)\, b_{5,4} = \frac{1}{120}. \tag{9.10}$$

The substitution of (9.8) into (9.10) after simplification yields:

$$w_4\, a_4\, b_{4,3} + w_5\, a_5\, b_{5,3} = \frac{a_4 - 2a_5 - 1}{120(a_4 - 1)}. \tag{9.10'}$$

Solving the system of equations (9.7) and (9.10′) for $w_4\, b_{4,3}$ and $w_5\, b_{5,3}$ we obtain:

$$w_4\, b_{4,3} = \frac{1}{120(a_4 - a_5)}\,, \tag{9.7′}$$

$$w_5\, b_{5,3} = \frac{3a_4 - 2a_5 - 1}{120(a_4 - 1)(a_5 - a_4)}\,. \tag{9.10″}$$

The substitution, respectively, from (9.4) and (9.5) into (9.7′) and (9.10″), after simplification, yields:

$$b_{4,3} = \tfrac{1}{2}\, a_4\, (1 - a_4)\, (2a_4 - 1)\,, \tag{9.7″}$$

$$b_{5,3} = \frac{a_5(a_5 - 1)(2a_5 - 1)(3a_4 - 2a_5 - 1)}{2(1 - a_4)}\,. \tag{9.10‴}$$

The operation (9.8) times (9.7″) gives:

$$w_5\, b_{4,3}\, b_{5,4} = -\frac{1}{120}\,.$$

The substitution of the latter into either one of the equations (7.13) or (7.14) yields:

$$\frac{1}{2}\, w_3 + w_4 \left(\frac{1}{2t}\, b_{4,2} + b_{4,3}\right) + w_5 \left[\frac{1}{2t}\, b_{5,2} + b_{5,3} + (b_{4,1} + b_{4,2})\, b_{5,4}\right] = \frac{1}{10}\,. \tag{9.13}$$

We thus replace (7.13) by (9.13) and discard (7.14) as dependent on equations (7.2) through (7.10) and (7.13).

Consider now the system of equations (7.6), (7.9) and (7.11). After the transposition of w_3's to the right side of these equations, the resulting system can be solved for w_2/t, $w_4\, (b_{4,1} + b_{4,2} + 2b_{4,3})$ and $w_5\, (b_{5,1} + b_{5,2} + 2b_{5,3} + 2a_4 \cdot b_{5,4})$ in terms of a_4, a_5 and w_3 or actually solely in terms of a_4 and a_5 since w_3 will be replaced by its equivalent expression as given in (9.3). We thus find:

$$\frac{w_2}{t} = \frac{2[10\, a_4 a_5 - 5(a_4 + a_5) + 3]}{15(2a_4 - 1)(2a_5 - 1)}\,, \tag{9.6′}$$

$$w_4\, (b_{4,1} + b_{4,2} + 2b_{4,3}) = \frac{a_4}{60(a_5 - a_4)(a_4 - 1)(2a_4 - 1)}\,, \tag{9.9}$$

(9.11) $$w_5 (b_{5,1} + b_{5,2} + 2b_{5,3} + 2a_4 b_{5,4}) = \frac{-a_5}{60(a_5 - a_4)(a_5 - 1)(2a_5 - 1)} .$$

The substitution, respectively, from (9.4) and (9.5) into (9.9) and (9.11), yields:

(9.9′) $$b_{4,1} + b_{4,2} + 2b_{4,3} = a_4^2 ,$$

(9.11′) $$b_{5,1} + b_{5,2} + 2b_{5,3} + 2a_4 b_{5,4} = a_5^2 .$$

The substitution of (9.9′) and (9.11′) in (7.12) gives:

$$\frac{1}{16\,t^2} w_2 + \frac{1}{4} w_3 + w_4 \frac{a_4^4}{4} + w_5 \frac{a_5^4}{4} = \frac{1}{20}$$

or

$$\frac{w_2}{4\,t^2} + w_3 + w_4\, a_4^4 + w_5\, a_5^4 = \frac{1}{5} .$$

Combining the latter equation with (7.5), we obtain

(9.12) $$\frac{w_2}{t^2} = \frac{1}{4} (w_1 + w_2) .$$

The substitution from (9.6′) and (9.2) into (9.12) gives:

$$\frac{2[10\, a_4 a_5 - 5(a_4 + a_5) + 3]}{15(2a_4 - 1)(2a_5 - 1)t} = \frac{10\, a_4 a_5 - 5(a_4 + a_5) + 3}{15(2\, a_5 - 1)(2a_4 - 1)}$$

or

(9.12′) $$t = 2.$$

Considering (9.12′) the equation (9.6′) can be written

(9.6″) $$w_2 = \frac{4[10\, a_4 a_5 - 5(a_4 + a_5) + 3]}{15(2a_4 - 1)(2a_5 - 1)} .$$

A comparison of (9.6″) with (9.2) yields

(9.2′) $$w_1 = 0 .$$

Consider now the equation (7.16) which can be written

$$\frac{1}{2t} w_5 b_{4,2} b_{5,4} = \frac{1}{60} - w_5 b_{4,3} b_{5,4} - \frac{1}{2} (w_4 b_{4,3} + w_5 b_{5,3}) .$$

We have found $t = 2$ and $w_5 b_{4,3} b_{5,4} = -1/120$. Substituting these values in the preceding equation and simplifying, we obtain:

$$w_5 b_{4,2} b_{5,4} = \frac{1}{10} - 2(w_4 b_{4,3} + w_5 b_{5,3}) . \tag{9.16}$$

Substituting from (9.7) and (9.8) into (9.16) and solving for $b_{4,2}$, we obtain

$$b_{4,2} = 2a_4 (2a_4 - 1) (3a_4 - 2) . \tag{9.16'}$$

The equation (9.9′) can be written

$$b_{4,1} = a_4^2 - b_{4,2} - 2b_{4,3} .$$

The substitution from (9.7″) and (9.16′) into the preceding equation yields

$$b_{4,1} = - a_4 (10 a_4^2 - 12 a_4 + 3) . \tag{9.9''}$$

We consider now (9.13). Substituting from (9.3), (9.4), (9.5), (9.7), (9.8), (9.12′), (9.16′) and (9.9″) into this equation and solving for $b_{5,2}$, we find after simplification:

$$b_{5,2} = \frac{2a_5(1 - 2a_5)(2a_5^2 - 8a_4 a_5 + a_5 + 6a_4 - 2)}{2a_4 - 1} . \tag{9.13'}$$

Finally, substituting from (9.8′), (9.10‴) and (9.13′) into (9.11′) and solving for $b_{5,1}$, we find

$$b_{5,1} = - a_5 (10 a_5^2 - 12 a_5 + 3) .$$

Now it is worthwhile observing that all the parameters present in the system of equations (7.1)-(7.16) have been determined as functions of a_4 and a_5; and this has been accomplished without the use of the equation (7.15). A check shows that these functions satisfy identically (7.15). Thus it can be concluded that the equation (7.15) can be discarded as dependent on other equations and that the totality of these functions constitute a solution set for the system (7.1)-(7.16).

Originally we had 16 equations and 21 parameters, to three of which we assigned numerical values and two others we made dependent on t. Thus we have eliminated two equations and five parameters leaving us with a system of 14 equations in 16 parameters. Hence, there was an excess of two parameters. This permited us to express 14 parameters in terms of the other two, i. e., a_4 and a_5.

Let us consider now the parameters which have been eliminated from the system (7.1)-(7.16), but are contained in (6). Three of these, namely $b_{2,1}$, $b_{3,1}$ and $b_{3,2}$, are still unknown but can be readily determined. In fact, since $t = 2$ we find

$$b_{2,1} = \frac{1}{2t} = \frac{1}{4}, \qquad b_{3,1} = 1 - t = -1, \qquad b_{3,2} = t = 2\,,$$

and consequently we have also

$$b_{2,0} = a_2 - b_{2,1} = \tfrac{1}{4}\,, \qquad b_{3,0} = a_3 - b_{3,1} - b_{3,2} = 0\,.$$

Thus all the parameters which figure in the formula (5 a) and in the set of incremental coefficients (5 b) have been determined. For convenience, they are grouped in the table below:

$$a_1 = a_2 = \frac{1}{2}\,, \qquad a_3 = 1\,,$$

$$b_{2,1} = b_{2,0} = \frac{1}{4}\,,$$

$$b_{3,2} = 2, \qquad b_{3,1} = -1, \qquad b_{3,0} = 0\,,$$

$$b_{4,3} = \frac{1}{2}\, a_4\, (1 - a_4)\, (2a_4 - 1)\,,$$

$$b_{4,2} = 2a_4\, (3a_4 - 2)\, (2a_4 - 1)\,,$$

$$b_{4,1} = -\, a_4\, (10\, a_4^2 - 12\, a_4 + 3),$$

$$b_{4,0} = a_4 - b_{4,1} - b_{4,2} - b_{4,3} = \frac{1}{2}\, a_4\, (2a_4 + 1)\, (1 - a_4)\,,$$

$$b_{5,4} = \frac{a_5(a_5 - 1)(2a_5 - 1)(a_5 - a_4)}{a_4(1 - a_4)(2a_4 - 1)}\,,$$

$$b_{5,3} = \frac{a_5(a_5 - 1)(2a_5 - 1)(3a_4 - 2a_5 - 1)}{2(1 - a_4)},$$

$$b_{5,2} = \frac{2a_5(1 - 2a_5)(2a_5^2 - 8a_4 a_5 + a_5 + 6a_4 - 2)}{2a_4 - 1},$$

$$b_{5,1} = -a_5 (10 a_5^2 - 12 a_5 + 3),$$

$$b_{5,0} = a_5 - b_{5,1} - b_{5,2} - b_{5,3} - b_{5,4},$$

$$w_5 = \frac{-1}{60 a_5(a_5 - a_4)(2a_5 - 1)(a_5 - 1)},$$

$$w_4 = \frac{1}{60 a_4(a_5 - a_4)(2a_4 - 1)(a_4 - 1)},$$

$$w_3 = \frac{10 a_4 a_5 - 10(a_4 + a_5) + 9}{60(a_4 - 1)(a_5 - 1)},$$

$$w_2 = \frac{4[10 a_4 a_5 - 5(a_4 + a_5) + 3]}{15(2a_5 - 1)(2a_4 - 1)},$$

$$w_1 = 0,$$

$$w_0 = 1 - w_2 - w_3 - w_4 - w_5.$$

Furthermore the previously indicated fourth order formula $\tilde{y}_4(x_0 + h)$ can now be determined. Using $t = 2$, we have

$$\tilde{y}_4(x_0 + h) = y_0 + \frac{1}{6}(k_0 + 4k_2 + k_3).$$

This completes the solution of our problem which was the determination of fifth order Runge-Kutta formulas with fourth order formulas imbedded in them.

4. – It is worthwhile observing that $b_{4,3}$, $b_{5,4}$, w_4 and w_5 can never vanish, while $b_{4,1}$ and $b_{5,1}$ vanish only if a_4 and a_5 take on the values $(6 \pm \sqrt{6})/10$, respectively. On the other hand either $b_{4,2}$ or $b_{4,0}$ will vanish if $a_4 = \frac{2}{3}$ or $a_4 = -\frac{1}{4}$, respectively.

The following six cases appear to be interesting:

I. $w_3 = 0$ and $a_4 = \frac{6}{10}$ $\left(\text{implying } a_5 = \frac{3}{4}\right)$,

II. $b_{5,2} = b_{5,3} = 0$ $\left(\text{implying } a_4 = \frac{8}{10},\ a_5 = \frac{7}{10}\right)$,

III. $b_{4,2} = b_{5,2} = 0$ $\left(\text{implying } a_4 = \frac{2}{3},\ a_5 = \frac{3}{2}\right)$,

IV. $b_{4,2} = w_2 = 0$ $\left(\text{implying } a_4 = \frac{2}{3},\ a_5 = \frac{2}{10}\right)$,

V. $b_{4,2} = w_3 = 0$ $\left(\text{implying } a_4 = \frac{2}{3},\ a_5 = \frac{7}{10}\right)$,

VI. $w_2 = w_3 = 0$ (implying $a_4 = (6 \pm \sqrt{6})/10,\ a_5 = (6 \mp \sqrt{6})/10)$.

They lead, respectively, to the six pseudo-iterative formulas listed below.

Formula I.

$$\tilde{y}_5(x_0 + h) = y_0 + 2k_2 + \frac{1}{54}(7k_0 - 125k_4 + 64k_5),$$

$k_0 = h\, f(x_0,\ y_0)$, $\tilde{y}_1(x_0 + h) = y_0 + k_0$,

$k_1 = h\, f(x_0 + 0.5\, h,\ y_0 + 0.5\, k_0)$, $\tilde{y}_2(x_0 + h) = y_0 + k_1$,

$k_2 = h\, f(x_0 + 0.5\, h,\ y_0 + 0.25\,(k_0 + k_1))$,

$k_3 = h\, f(x_0 + h,\ y_0 - k_1 + 2k_2)$, $\tilde{y}_4(x_0 + h) = y_0 + \frac{1}{6}(k_0 + 4k_2 + k_3)$,

$k_4 = h\, f(x_0 + 0.6\, h,\ y_0 + 0.024(11k_0 + 15k_1 - 2k_2 + k_3))$,

$k_5 = h\, f(x_0 + 0.75\, h,\ y_0 + 0.01171875(18k_0 + 24k_1 + 40k_2 + 7k_3 - 25k_4))$.

Note that $0.01171875 = 3/256$.

Formula II.

$$\tilde{y}_5(x_0+h) = y_0 + \frac{1}{504}(69k_0 + 616k_2 - 56k_3 + 875k_4 - 1000k_5)\,,$$

$$\left.\begin{aligned} k_0 &= \\ k_1 &= \\ k_2 &= \\ k_3 &= \end{aligned}\right\}\ \text{Same as in Formula I,}$$

$$k_4 = h\,f(x_0 + 0.8\,h\,,\ y_0 + 0.016(13k_0 + 10k_1 + 24k_2 + 3k_3))\,,$$

$$k_5 = h\,f(x_0 + 0.7\,h\,,\ y_0 + 0.0875(3k_0 + 4k_1 + k_4))\,.$$

Note that 0.0875 = 7/80.

Formula III.

$$\tilde{y}_5(x_0+h) = y_0 + 0.15\,k_0 - 0.27\,k_4 + \frac{1}{75}(65k_2 + 20k_3 - k_5)\,,$$

$$\left.\begin{aligned} k_0 &= \\ k_1 &= \\ k_2 &= \\ k_3 &= \end{aligned}\right\}\ \text{Same as in Formula I ,}$$

$$k_4 = h\,f\left(x_0 + \frac{2}{3}h\,,\ y_0 + \frac{1}{27}(7k_0 + 10k_1 + k_3)\right),$$

$$k_5 = h\,f(x_0 + 1.5\,h\,,\ y_0 + 0.375(k_0 - 30k_1 - 12k_3 + 45k_4))\,.$$

Note that 0.375 = 3/8.

Formula IV.

$$\tilde{y}_5(x_0+h) = y_0 + \frac{1}{336}(14k_0 + 35k_3 + 162k_4 + 125k_5),$$

$$\left.\begin{array}{l} k_0 = \\ k_1 = \\ k_2 = \\ k_3 = \end{array}\right\} \text{Same as in Formula I,}$$

$$k_4 = h\,f\left(x_0 + \frac{2}{3}h,\ \ y_0 + \frac{1}{27}(7k_0 + 10k_1 + k_3)\right),$$

$$k_5 = h\,f(x_0 + 0.2\,h\,,\ y_0 + 0.0016(28k_0 - 125k_1 + \\ + 546k_2 + 54k_3 - 378k_4)).$$

Formula V.

$$\tilde{y}_5(x_0+h) = y_0 + \frac{1}{84}(11k_0 + 140k_2 - 567k_4 + 500k_5),$$

$$\left.\begin{array}{l} k_0 = \\ k_1 = \\ k_2 = \\ k_3 = \end{array}\right\} \text{Same as in Formula I ,}$$

$$k_4 = h\,f\left(x_0 + \frac{2}{3}h,\ \ y_0 + \frac{1}{27}(7k_0 + 10k_1 + k_3)\right),$$

$$k_5 = h\,f(x_0 + 0.7\,h\,,\ y_0 + 0.2478\,k_0 + 0.35\,k_1 + \\ + 0.0896\,k_2 + 0.0504\,k_3 - 0.0378\,k_4),$$

or

$$k_5 = h\,f(x_0 + 0.7\,h\,,\ y_0 + 0.014(177k_0 + 250k_1 + \\ + 64k_2 + 36k_3 - 27k_4)).$$

Formula VI.

$$\tilde{y}_5(x_0+h) = y_0 + \frac{1}{36}[4k_0 + (16+\sqrt{6})\,k_4 + (16-\sqrt{6})\,k_5]\,,$$

$$\left.\begin{aligned} k_0 &= \\ k_1 &= \\ k_2 &= \\ k_3 &= \end{aligned}\right\} \text{Same as in Formula I}\,,$$

$$\begin{aligned} k_4 &= h\,f(x_0 + 0.1(6-\sqrt{6})\,h,\ y_0 + \\ &\qquad + 0.002[(93+2\sqrt{6})k_0 + 4(56-11\sqrt{6})k_2 + (3-8\sqrt{6})k_3]), \\ k_5 &= h\,f(x_0 + 0.1(6+\sqrt{6})h\,,\ y_0 + \\ &\qquad + 0.0004[9(29-6\sqrt{6})\,k_0 + 4(123-47\sqrt{6})k_2 + \\ &\qquad\qquad + (363-32\sqrt{6})k_3 + 4(96+131\sqrt{6})\,k_4])\,. \end{aligned}$$

It is worthwhile observing that in the latter formula $w_1 = w_2 = w_3 = b_{3,0} = b_{4,1} = b_{5,1} = 0$.

5. – It is known that the complete solution of the system of algebraic equations associated with fourth order Runge-Kutta method is composed of four distinct solution sets [4]. One of these, which may be called the general solution, gives six parameters, from the totality of eight parameters involved in the method, as functions of a_1 and a_2 . The other three sets, which may be referred to as singular solutions, give seven of the eight parameters as function of a single parameter which is usually taken as $b_{3,2} = t \neq 0$. In the first part of this work we used one of these singular solution sets. We shall investigate now the remaining two sets.

In the first four stages of (5 b) let

$$(10)\qquad a_1 = a_3 = 1\,,\qquad a_2 = \frac{1}{2}\,,\qquad b_{2,1} = \frac{1}{8}\,,$$

$$b_{2,0} = \frac{1}{2} - \frac{1}{8} = \frac{3}{8}\,,\qquad b_{3,2} = t\,,\qquad b_{3,1} = -\frac{t}{4}\,,$$

$$b_{3,0} = 1 + \frac{t}{4} - t = 1 - \frac{3}{4}t\,.$$

Then at the fourth stage of (5 b) the use of the formula

$$\tilde{y}_4(x_0 + h) = y_0 + \frac{1}{6}\left[k_0 + \frac{t-2}{t} k_1 + 4k_2 + \frac{2}{t} k_3\right]$$

will give a fourth order approximation to $y(x_0 + h)$.

Thus we assign now the parameters a_i $(i = 1, 2, 3)$, $b_{2,1}$, $b_{3,1}$, $b_{3,2}$ of the system of algebraic equations (I-XVI) the values as indicated in (10). The resulting new system is as follows:

(11.1) $$w_0 + w_1 + w_2 + w_3 + w_4 + w_5 = 1\,,$$

(11.2) $$(w_1 + w_3) + \frac{1}{2} w_2 + w_4\, a_4 + w_5\, a_5 = \frac{1}{2}\,,$$

(11.3) $$(w_1 + w_3) + \frac{1}{4} w_2 + w_4\, a_4^2 + w_5\, a_5^2 = \frac{1}{3}\,,$$

(11.4) $$(w_1 + w_3) + \frac{1}{8} w_2 + w_4\, a_4^3 + w_5\, a_5^3 = \frac{1}{4}\,,$$

(11.5) $$(w_1 + w_3) + \frac{1}{16} w_2 + w_4\, a_4^4 + w_5\, a_5^4 = \frac{1}{5}\,,$$

(11.6) $$\left[\frac{1}{8} w_2 - \frac{1}{4} t\, w_3 + w_4\,(b_{4,1} + b_{4,3}) + w_5\,(b_{5,1} + b_{5,3})\right] + \\ + \frac{1}{2}\left[(w_3\, t + w_4\, b_{4,2} + w_5\, b_{5,2})\right] + a_4\,[w_5\, b_{5,4}] = \frac{1}{6}\,,$$

(11.7) $$\left[\frac{1}{8} w_2 - \frac{1}{4} t\, w_3 + w_4\,(b_{4,1} + b_{4,3}) + w_5\,(b_{5,1} + b_{5,3})\right] + \\ + \frac{1}{4}\left[(w_3\, t + w_4\, b_{4,2} + w_5\, b_{5,2})\right] + a_4^2\,[w_5\, b_{5,4}] = \frac{1}{12}\,,$$

(11.8) $$\left[\frac{1}{8} w_2 - \frac{1}{4} t\, w_3 + w_4\,(b_{4,1} + b_{4,3}) + w_5\,(b_{5,1} + b_{5,3})\right] + \\ + \frac{1}{8}\left[(w_3\, t + w_4\, b_{4,2} + w_5\, b_{5,2})\right] + a_4^3\,[w_5\, b_{5,4}] = \frac{1}{20}\,;$$

(11.9) $$\frac{1}{16} w_2 + \frac{1}{4} w_3\, t + w_4\, a_4\left(b_{4,1} + \frac{1}{2} b_{4,2} + b_{4,3}\right) + \\ + w_5\, a_5\left(b_{5,1} + \frac{1}{2} b_{5,2} + b_{5,3} + a_4\, b_{5,4}\right) = \frac{1}{8}\,,$$

$$(11.10) \qquad \frac{1}{16} w_2 + 0 w_3 t + w_4 a_4 \left(b_{4,1} + \frac{1}{4} b_{4,2} + b_{4,3} \right) + \\ + w_5 a_5 \left(b_{5,1} + \frac{1}{4} b_{5,2} + b_{5,3} + a_4^2 b_{5,4} \right) = \frac{1}{15},$$

$$(11.11) \qquad \frac{1}{32} w_2 + \frac{1}{4} w_3 t + w_4 a_4^2 \left(b_{4,1} + \frac{1}{2} b_{4,2} + b_{4,3} \right) + \\ + w_5 a_5^2 \left(b_{5,1} + \frac{1}{2} b_{5,2} + b_{5,3} + a_4 b_{5,4} \right) = \frac{1}{10},$$

$$(11.12) \qquad \frac{1}{64} w_2 + \frac{1}{16} w_3 t^2 + w_4 \left(b_{4,1} + \frac{1}{2} b_{4,2} + b_{4,3} \right)^2 + \\ + w_5 \left(b_{5,1} + \frac{1}{2} b_{5,2} + b_{5,3} + a_4 b_{5,4} \right)^2 = \frac{1}{20},$$

$$(11.13) \qquad \frac{1}{8} w_3 t + w_4 \left[\frac{1}{8} b_{4,2} + \frac{1}{4} t b_{4,3} \right] + \\ + w_5 \left[\frac{1}{8} b_{5,2} + \frac{1}{4} t b_{5,3} + \left(b_{4,1} + \frac{1}{2} b_{4,2} + b_{4,3} \right) b_{5,4} \right] = \frac{1}{24},$$

$$(11.14) \qquad \frac{1}{8} w_3 t + \frac{1}{8} w_4 b_{4,2} + w_5 \left[\frac{1}{8} b_{5,2} + \left(b_{4,1} + \frac{1}{4} b_{4,2} + b_{4,3} \right) b_{5,4} \right] = \frac{1}{60},$$

$$(11.15) \qquad \frac{3}{16} w_3 t + w_4 \left[\frac{1}{8} \left(\frac{1}{2} + a_4 \right) b_{4,2} + \frac{1}{4} (1 + a_4) t b_{4,3} \right] + w_5 \left[\frac{1}{8} \left(\frac{1}{2} + a_5 \right) b_{5,2} + \\ + \frac{1}{4} (1 + a_5) t b_{5,3} + (a_4 + a_5) \left(b_{4,1} + \frac{1}{2} b_{4,2} + b_{4,3} \right) b_{5,4} \right] = \frac{7}{120},$$

$$(11.16) \qquad w_4 b_{4,3} t + w_5 [b_{5,3} t + (b_{4,2} + 2t b_{4,3}) b_{5,4}] = \frac{1}{15}.$$

At first approach it appears again that we are dealing with a tight case, since this complex system is composed of 16 algebraic equations in 16 unknowns. However, as in the preceding case we shall end up with 14 independent equations in 16 unknowns. This will permit the determination of 14 parameters as functions of a_4 and a_5.

The system of four equations (11.2)-(11.5) is solvable for $w_1 + w_3$, w_2, w_4 and w_5 provided that

$$D = \begin{vmatrix} 1 & \frac{1}{2} & a_4 & a_5 \\ 1 & \frac{1}{4} & a_4^2 & a_5^2 \\ 1 & \frac{1}{8} & a_4^3 & a_5^3 \\ 1 & \frac{1}{16} & a_4^4 & a_5^4 \end{vmatrix} \neq 0 .$$

The latter being a VANDERMONDE determinant, one readily finds:

$$D = -\frac{1}{4} a_4 a_5 (a_5 - a_4) \left(a_5 - \frac{1}{2}\right) (a_5 - 1) \left(a_4 - \frac{1}{2}\right) (a_4 - 1) .$$

Thus assuming

(12) $a_4 \neq a_5$ and $a_i \neq 0$, $a_i - 1 \neq 0$, $a_i - \frac{1}{2} \neq 0$, $(i = 4, 5)$,

we find

(13.2) $$w_1 + w_3 = \frac{10 a_4 a_5 - 10(a_4 + a_5) + 9}{60(a_5 - 1)(a_4 - 1)},$$

(13.3) $$w_2 = \frac{4[10 a_4 a_5 - 5(a_4 + a_5) + 3]}{15(2a_5 - 1)(2a_4 - 1)},$$

(13.4) $$w_4 = \frac{1}{60 a_4 (a_5 - a_4)(2a_4 - 1)(a_4 - 1)} \neq 0,$$

(13.5) $$w_5 = \frac{-1}{60 a_5 (a_5 - a_4)(2a_5 - 1)(a_5 - 1)} \neq 0.$$

Solving the system of three equations (11.6)-(11.8) for the quantities in brackets we find:

(13.6) $$\frac{1}{8} w_2 - \frac{1}{4} w_3 t + w_4 (b_{4,1} + b_{4,3}) + w_5 (b_{5,1} + b_{5,3}) = \frac{1}{60(1 - a_4)},$$

$$w_3\,t + w_4\,b_{4,2} + w_5\,b_{5,2} = \frac{2(5a_4 - 2)}{15(2a_4 - 1)}, \tag{13.7}$$

$$w_5\,b_{5,4} = \frac{1}{60\,a_4\,(a_4 - 1)(2a_4 - 1)}. \tag{13.8}$$

The combination of (13.5) and (13.8) gives

$$b_{5,4} = -\frac{a_5\,(a_5 - a_4)(2a_5 - 1)(a_5 - 1)}{a_4(a_4 - 1)(2a_4 - 1)}. \tag{13.8'}$$

The subtraction of (11.10) from (11.9) yields:

$$w_3\,t + w_4\,b_{4,2}\,a_4 + w_5\,b_{5,2}\,a_5 = \frac{2\,a_5 + 14\,a_4 - 7}{30(2a_4 - 1)}. \tag{13.10}$$

The equations (11.6), (11.9) and (11.11) may be written

$$\frac{1}{4}[w_3\,t] + \left[w_4\left(b_{4,1} + \frac{1}{2}b_{4,2} + b_{4,3}\right)\right] + \left[w_5\left(b_{5,1} + \frac{1}{2}b_{5,2} + b_{5,3} + a_4\,b_{5,4}\right)\right] = \frac{1}{6} - \frac{1}{8}w_2,$$

$$\frac{1}{4}[w_3\,t] + a_4\left[w_4\left(b_{4,1} + \frac{1}{2}b_{4,2} + b_{4,3}\right)\right] + a_5\left[w_5\left(b_{5,1} + \frac{1}{2}b_{5,2} + b_{5,3} + a_4\,b_{5,4}\right)\right] = \frac{1}{8} - \frac{1}{16}w_2,$$

$$\frac{1}{4}[w_3\,t] + a_4^2\left[w_4\left(b_{4,1} + \frac{1}{2}b_{4,2} + b_{4,3}\right)\right] + a_5^2\left[w_5\left(b_{5,1} + \frac{1}{2}b_{5,2} + b_{5,3} + a_4\,b_{5,4}\right)\right] = \frac{1}{10} - \frac{1}{32}w_2.$$

This system is solvable for the quantities in brackets if

$$\begin{vmatrix} \frac{1}{4} & 1 & 1 \\ \frac{1}{4} & a_4 & a_5 \\ \frac{1}{4} & a_4^2 & a_5^2 \end{vmatrix} = \frac{1}{4}(a_5 - a_4)(a_5 - 1)(a_4 - 1) \neq 0\,.$$

In view of (12) this condition being satisfied, we find:

(13.6′) $$w_3\, t = \frac{10\, a_4\, a_5 - 10(a_4 + a_5) + 9}{30(a_5 - 1)(a_4 - 1)},$$

(13.9′) $$\begin{cases} w_4 \left(b_{4,1} + \frac{1}{2}\, b_{4,2} + b_{4,3}\right) = \dfrac{a_4}{120\,(a_5 - a_4)(a_4 - 1)(2a_5 - 1)} \\ \text{or} \qquad b_{4,1} + \frac{1}{2}\, b_{4,2} + b_{4,3} = \frac{1}{2}\, a_4^2, \end{cases}$$

(13.11′) $$\begin{cases} w_5 \left(b_{5,1} + \frac{1}{2}\, b_{5,2} + b_{5,3} + a_4\, b_{5,4}\right) = \dfrac{-\,a_5}{120(a_5 - a_4)(a_5 - 1)(2a_5 - 1)} \\ \text{or} \qquad b_{5,1} + \frac{1}{2}\, b_{5,2} + b_{5,3} + a_4\, b_{5,4} = \frac{1}{2}\, a_5^2\,. \end{cases}$$

The substitution from (13.9′) and (13.11′) into (11.12), yields

$$\frac{1}{16}\, w_2 + \frac{1}{4}\, w_3\, t^2 + w_4\, a_4^4 + w_5\, a_5^4 = \frac{1}{5}\,.$$

The combination of the latter with (11.5) gives

(13.12′) $$\frac{1}{4}\, w_3\, t^2 = w_1 + w_3\,.$$

Substituting from (13.2) and (13.6′) into (13.12′) we find

(13.12″) $$t = 2\,.$$

Considering the latter, (13,6′) becomes

(13.6″) $$w_3 = \frac{10\, a_4\, a_5 - 10(a_4 + a_5) + 9}{60(a_5 - 1)(a_4 - 1)}\,.$$

The comparison of (13.2) and (13.6″) gives

(13.2′) $$w_1 = 0\,.$$

We consider now the equations (13.7) and (13.10); we may write

$$[w_4\, b_{4,2}] + [w_5\, b_{5,2}] = \frac{2(5a_4 - 2)}{15(2a_4 - 1)} - 2w_3\,,$$

$$[w_4\, b_{4,2}]\, a_4 + [w_5\, b_{5,2}]\, a_5 = \frac{2a_5 + 14a_4 - 7}{30(2a_4 - 1)} - 2w_3\,.$$

Solving for the quantities in brackets we obtain:

(13.7′) $$w_4\, b_{4,2} = \frac{3a_4 - 2}{30(a_5 - a_4)(a_4 - 1)}$$

or

(13.7″) $$b_{4,2} = 2a_4\,(3a_4 - 2)\,(2a_4 - 1)\,,$$

(13.10′) $$w_4\, b_{5,2} = \frac{2a_5^2 - 8a_4\, a_5 + a_5 + 6a_4 - 2}{30(a_5 - a_4)(2a_4 - 1)(a_5 - 1)}$$

or

(13.10″) $$b_{5,2} = -\frac{2a_5(2a_5 - 1)(2a_5^2 - 8a_4a_5 + a_5 + 6a_4 - 2)}{2a_4 - 1}\,.$$

It must now be observed that the equation (11.14) can be constructed by the linear combination of (13.7), (13.8), (13.9′) and (13.7″). Thus (11.14) should not be considered as an independent equation.

The subtraction of (11.14) from (11.13) yields

(13.13) $$w_4\, t\, b_{4,3} + w_5\, t\, b_{5,3} + w_5\, b_{4,2}\, b_{5,4} = \frac{1}{10}\,.$$

The subtraction of (11.13′) from (11.16) yields

$$2w_5\, t\, b_{4,3}\, b_{5,4} = -\frac{1}{30}\,.$$

Substituting from (13.8) and (13.12″) into (11.16′), we obtain

(13.16) $$b_{4,3} = -\frac{1}{2}\, a_4\,(a_4 - 1)\,(2a_4 - 1) \neq 0\,.$$

Substituting from (13.4), (13.5), (13.8), (13.12″), (13.7′) and (13.16) into (13.13), we find

(13.13′) $$b_{5,3} = \frac{a_5(2a_5 - 1)(a_5 - 1)(2a_5 - 3a_4 + 1)}{2(a_4 - 1)}\,.$$

The parameters $b_{4,2}$, $b_{4,3}$ and $b_{5,2}$, $b_{5,3}$, $b_{5,4}$ have been determined as functions of a_4 and a_5. The substitution of these appropriate functions in (13.9′) and (13.11′) yields

$$b_{4,1} = -\frac{1}{2} a_4 (10\, a_4^2 - 12\, a_4 + 3) ,$$

$$b_{5,1} = -\frac{1}{2} a_5 (10\, a_5^2 - 12\, a_5 + 3) .$$

On noting that $t = 2$, the parameters $b_{3,1}$ and $b_{3,2}$ in (10) and the formula giving $\tilde{y}_4(x_0 + h)$ become

$$b_{3,1} = -\frac{1}{2} , \qquad b_{3,2} = 2 ,$$

$$\tilde{y}_4(x_0 + h) = y_0 + \frac{1}{6} (k_0 + 4k_2 + k_3) .$$

We note that all the parameters present in the system of equations (11.1)-(11.16) have been determined as functions of a_4 and a_5 and yet the equation (11.15) has never been used in this process. A check shows that these functions satisfy identically (11.15). Thus (11.15) like (11.14) is not an independent equation. This gives us an excess of two parameters over the number of independent equations. As indicated before, this excess permits the expression of parameters in terms of a_4 and a_5.

For convenience these parameters are listed in the following table:

$$a_1 = a_3 = 1 , \qquad a_2 = \frac{1}{2} ,$$

$$b_{2,1} = \frac{1}{8} , \qquad b_{2,0} = \frac{3}{8} ,$$

$$b_{3,2} = 2 , \qquad b_{3,1} = -\frac{1}{2} , \qquad b_{3,0} = -\frac{1}{2} ,$$

$$b_{4,3} = -\frac{1}{2} a_4 (a_4 - 1) (2a_4 - 1) \neq 0 ,$$

$$b_{4,2} = 2\, a_4 (3\, a_4 - 2) (2\, a_4 - 1) ,$$

$$b_{4,1} = -\frac{1}{2} a_4 (10\, a_4^2 - 12\, a_4 + 3),$$

$$b_{4,0} = a_4 - b_{4,1} - b_{4,2} - b_{4,3},$$

$$b_{5,4} = -\frac{a_5(a_5 - a_4)(2a_5 - 1)(a_5 - 1)}{a_4(a_4 - 1)(2a_4 - 1)} \neq 0,$$

$$b_{5,3} = \frac{a_5(2a_5 - 1)(a_5 - 1)(2a_5 - 3a_4 + 1)}{2(a_4 - 1)},$$

$$b_{5,2} = -\frac{2a_5(2a_5 - 1)(2a_5^2 - 8a_4 a_5 + a_5 + 6a_4 - 2)}{2a_4 - 1},$$

$$b_{5,1} = -\frac{1}{2} a_5 (10\, a_5^2 - 12\, a_5 + 3),$$

$$b_{5,0} = a_5 - b_{5,1} - b_{5,2} - b_{5,3} - b_{5,4},$$

$$w_5 = \frac{-1}{60\, a_5(a_5 - a_4)(a_5 - 1)(2a_5 - 1)} \neq 0,$$

$$w_4 = \frac{1}{60\, a_4(a_5 - a_4)(a_4 - 1)(2a_4 - 1)} \neq 0,$$

$$w_3 = \frac{10\, a_4 a_5 - 10(a_4 + a_5) + 9}{60(a_5 - 1)(a_4 - 1)},$$

$$w_2 = \frac{4[10\, a_4 a_5 - 5(a_4 + a_5) + 3]}{15(2a_5 - 1)(2a_4 - 1)},$$

$$w_1 = 0,$$

$$w_0 = 1 - w_2 - w_3 - w_4 - w_5 .$$

It is seen that the above set of coefficients is quite similar to the one found in the preceding case since only the coefficients with subscript 1 and 0 such as a_1, $a_{2,1}$, $b_{2,0}$, etc. are different. Then evidently the present formulas will differ little from the formulas of the preceding case (for the same values of a_4 and a_5), but since they contain one additional « k » in their fourth stage, it is reasonable to expect that they may provide approximations which are somewhat less accurate than others.

At any rate all fifth order pseudo-iterative formulas of the present case have the form:

$$k_0 = h\,f(x_0\,,\ y_0)\,, \qquad \tilde{y}_1(x_0+h) = y_0 + k_0\,,$$

$$k_1 = h\,f(x_0+h,\ y_0+k_0)\,, \qquad \tilde{y}_2(x_0+h) = y_0 + \frac{1}{2}(k_0+k_1),$$

$$k_2 = h\,f\left(x_0+\frac{1}{2}h,\ y_0+\frac{1}{8}(3k_0+k_1)\right),$$

$$k_3 = h\,f\left(x_0+h,\ y_0-\frac{1}{2}(k_0+k_1-4\,k_2)\right), \qquad \tilde{y}_4(x_0+h) = y_0+\frac{1}{6}(k_0+4k_2+k_3)\,,$$

$$k_4 = h\,f(x_0+a_4\,h,\ y_0+\sum_0^3 b_{4,i}\,k_i)\,,$$

$$k_5 = h\,f(x_0+a_5\,h,\ y_0+\sum_0^4 b_{5,i}\,k_i)\,, \qquad \tilde{y}_5\,(x_0+h) = y_0+w_0\,k_0+\sum_2^5 w_i\,k_i\,,$$

where as it is seen $w_1 = 0$.

6. – We now consider the last of the three singular solution sets of the fourth order method, and let, in the first four stages of (5 b),

$$(14)\quad a_1 = \frac{1}{2}\,, \qquad a_2 = 0\,, \qquad a_3 = 1\,, \qquad b_{2,1} = \frac{1}{2t}\,, \qquad b_{3,1} = \frac{3}{2}\,, \qquad b_{3,2} = t \neq 0\,.$$

Then at the fourth stage of (5 b) the use of the formula

$$\tilde{y}_4(x_0+h) = y_0 + \frac{1}{6}\left[(1-t)\,k_0 + 4\,k_1 + t\,k_2 + k_3\right]$$

will provide a fourth order approximation to $y(x_0+h)$.

The substitution from (14) into the sixteen algebraic equations (I-XVI) yields a new system of algebraic equations. Following a method more or less similar to the ones used in the preceding two cases one finds, after much tedious work, that this system has no solution.

7. – In Formula I we have $w_1 = w_3 = b_{3,0} = 0$. This leaves 18 non-zero coefficients (out of 21 coefficients) and for this reason we shall say that this formula involves 18 k's.

The four Formulas II-V involve 17 k's each while the Formula VI involves only 15 k's. In spite of this, the latter formula may yield unsatisfactory results. This is due to the fact that most of its coefficients are irrationals.

The five Formulas I-V exhibit various advantages relative to each other. For instance Formulas I and II each have only one inexact coefficient, $\frac{1}{54}$ and $\frac{1}{504}$, respectively. However, Formula I has one more « k » than Formula II. On the other hand k_5 which constitutes the last stage of any fifth order formula, inherits errors from the preceding 5 stages or k's and for this reason it is preferable to attach to it a small weight-factor ($|w_5|$). From this standpoint, Formula I is better than Formula II, and Formula IV is the best of all since the corresponding weight-factors for I, II and IV are $\frac{64}{54} \approx 1.18$, $\frac{1000}{504} \approx 1.98$ and $\frac{125}{336} \approx 0.37$.

Note that in the classical NYSTROM's fifth order formula $w_5 = 125/192 \approx 0.65$. For the sake of completeness as well as for the convenience of the reader this formula is given below:

$$\tilde{y}_5(x_0 + h) = y_0 + \frac{1}{192}(23\,k_0 + 125\,k_2 - 81\,k_4 + 125\,k_5),$$

where:

$$k_0 = h\,f(x_0\,,\ y_0)\,,$$

$$k_1 = h\,f\left(x_0 + \frac{1}{3}h\,,\ y_0 + \frac{1}{3}k_0\right),$$

$$k_2 = h\,f\left(x_0 + \frac{2}{5}h\,,\ y_0 + \frac{1}{25}(4\,k_0 + 6\,k_1)\right),$$

$$k_3 = h\,f\left(x_0 + h\,,\ y_0 + \frac{1}{4}(k_0 - 12\,k_1 + 15\,k_2)\right),$$

$$k_4 = h\,f\left(x_0 + \frac{2}{3}h\,,\ y_0 + \frac{1}{81}(6\,k_0 + 90\,k_1 - 50\,k_2 + 8\,k_3)\right),$$

$$k_5 = h\,f\left(x_0 + \frac{4}{5}h\,,\ y_0 + \frac{1}{75}(6\,k_0 + 36\,k_1 + 10\,k_2 + 8\,k_3)\right).$$

For the purpose of illustration we consider the boundary value problems:

$$\begin{cases} \dfrac{dy}{dx} = \dfrac{m\,y}{x+1} & (m = 1,\ 2,\ 5) \\ x_0 = 0, \qquad y_0 = 1\,, \end{cases}$$

which have as solutions $y = (x+1)^m$ and are representative of an infinite variety of cases or problems.

We shall determine through a single application of the Formula IV the approximations $\tilde{y}_4(x_0 + h)$ and $\tilde{y}_5(x_0 + h)$, where $h = 2^{-n}$ $(n = 0,\ 1,\ \ldots,\ 15)$.

The results which are listed in the various tables below were obtained through an IBM 7094 computer by using double precision (computations made to 16 figures and final results rounded to 12 figures). For comparison are also listed the exact values and fifth order approximations obtained by the use of NYSTROM's formula.

Problem: $\dfrac{dy}{dx} = \dfrac{y}{x+1}$ with (0, 1).

$h = 2^{-n}$	Solutions	
$n = 0$	2.000 000 000 00	Formula IV (imbedded) 4th order
	2.000 000 000 36	Formula IV 5th order
	2.000 000 002 25	NYSTROM
	2.000 000 000 00	Exact value
$n = 1$	1.500 000 000 00	Formula IV (imbedded) 4th order
	1.500 000 000 10	Formula IV 5th order
	1.500 000 000 65	NYSTROM
	1.500 000 000 00	Exact value
$n = 2$	1.250 000 000 00	Formula IV (imbedded) 4th order
	1.250 000 000 03	Formula IV 5th order
	1.250 000 000 18	NYSTROM
	1.250 000 000 00	Exact value
$n = 3$	1.125 000 000 00	Formula IV (imbedded) 4th order
	1.125 000 000 01	Formula IV 5th order
	1.125 000 000 05	NYSTROM
	1.125 000 000 00	Exact value
$n = 4$	1.062 500 000 00	Formula IV (imbedded) 4th order
	1.062 500 000 00	Formula IV 5th order
	1.062 500 000 01	NYSTROM
	1.062 500 000 00	Exact value
$n = 5$	1.031 250 000 00	Same for all four methods
$n = 6$	1.015 625 000 00	» » » » »
$n = 7$	1.007 812 500 00	» » » » »
$n = 8$	1.003 906 250 00	» » » » »
$n = 9$	1.001 953 125 00	» » » » »
$n = 10$	1.000 976 562 50	» » » » »
$n = 11$	1.000 488 281 25	» » » » »
$n = 12$	1.000 244 140 63	» » » » »
$n = 13$	1.000 122 070 31	» » » » »
$n = 14$	1.000 061 035 16	» » » » »
$n = 15$	1.000 030 517 58	» » » » » .

It is seen that, for $h = 1, \frac{1}{2}, \frac{1}{4}$ and $\frac{1}{8}$, the approximations provided by the fourth order formula are better than those of the two fifth orders. This may appear as paradoxical at first but it has a simple explanation. In fact in this problem the truncation errors related to RUNGE-KUTTA type formulas are nil **[8]**. It follows that the discrepancies between the exact values and the values given by the indicated formulas are due solely to round-off errors. Since the fifth order formulas are much more complex than the fourth order formula the round-off errors associated with them are much greater.

To be more specific the fourth order formula is of four stages (requires four substitutions), has eight k's and involves one inexact coefficient which is 1/6. The two fifth order formulas are of six stages (require six substitutions) have either 17 or 18 k's and involve either three or four inexact coefficients $\left(\frac{2}{3}, \frac{1}{27}, \frac{1}{336}\right.$, or $\left.\frac{1}{3}, \frac{1}{3}, \frac{2}{3}, \frac{1}{81}, \frac{1}{75}, \frac{1}{192}\right)$ according to whether we consider the Formula IV or NYSTROM's formula, respectively. These characteristics indicate that Formula IV will contribute less to the generation of round-off errors than NYSTROM's formula. And above computed results confirm this expectation since with $h = 1$ the round-off error originated from NYSTROM's formula is 6.25 (= 225/36) times larger than that originated from Formula IV. With $h = \frac{1}{2}, \frac{1}{4}$ and $\frac{1}{8}$ the corresponding round-off ratios become 6.5, 6 and 5, respectively.

It is worthwhile mentioning that if the sixth stage of Formula IV is written in the equivalent form of

$$k_5 = h\, f(x_0 + 0.2\, h, \quad y_0 - 0.2\, k_1 + 0.0032\, (14\, k_0 + 273\, k_2 + 27\, k_3 - 189\, k_4)),$$

then the round-off error in $\tilde{y}_5(x_0 + h)$ resulting from the use of this different version of Formula IV is about doubled when $h = 1, \frac{1}{2}$ and $\frac{1}{4}$.

On the other hand, the use of Formula VI involving irrational coefficients yields when $h = 1$:

$$\tilde{y}_5(x_0 + h) = 2.019\,145\,217\,65.$$

The round-off error associated with this value is 53 million times larger than that associated with Formula IV. As step-length « h » decreases the round-off errors decrease in magnitude and only when we reach the step-length $h = 1/65536$ does this formula (VI) start to yield the exact values. With Formula IV we begin to obtain exact values with a step-length considerably larger (precisely 4096 times) since in this case $h = 1/16$.

As far as the problem of estimation of errors is concerned we use the rule described earlier. For instance with $h = 1$ we found

$$\tilde{y}_4 = 2.000\,000\,000\,\underline{00}\,, \qquad \tilde{y}_5 = 2.000\,000\,000\,\underline{36}\,.$$

These two values being in agreement with each other up to their 9-th decimal figure, we consider either $\tilde{y}_5$ to have 9 decimal figures in agreement with the exact value or 10^{-9} to be an upper bound for the committed error. We note that either one of these considerations is true. We may also write $\tilde{y}_5 = 2\,000\,000\,000$ and accept this value as an approximation correct to 9 decimal figures.

The application of this rule to any entry in the above table always leads to correct results.

This rule gives satisfactory results also in the case where a pseudo-iterative formula is repeatedly applied over an extended interval. For instance in the considered problem we find as an approximation for $y(1) = 2$ the following:

with $h = 1/2$:	$2.000\,000\,000\,\underline{13}$	4th order Formula IV
	$2.000\,000\,000\,\underline{20}$	5th order Formula IV,
$h = 1/4$:	$2.000\,000\,000\,09$	4th order Formula IV
	$2.000\,000\,000\,10$	5th order Formula IV,
$h = 1/8$:	$2.000\,000\,000\,05$	4th order Formula IV
	$2.000\,000\,000\,05$	5th order Formula IV.

Thus in the case where $h = \frac{1}{2}$ or $h = \frac{1}{4}$ the rule or method indicates that the computed fifth order approximations have 9 decimal figures in agreement with the exact value, which is true.

However, when $h = \frac{1}{8}$, $\tilde{y}_4 = \tilde{y}_5$. In this instance it must be taken into consideration that the last figure of these approximations, which is 5, is obtained through a rounding operation. For this reason we shall exclude this last figure in counting the leading decimal digits in agreement and consider $\tilde{y}_5 = 2.000\,000\,000\,05$ as having only 10 leading decimal figures in agreement with the exact value.

This latter observation is valid for all other approximations, listed below in the table, for which $h \leq 1/16$.

$h = 2^{-n}$	Approximations	for $y(1) = 2$
$n = 0$	2.000 000 000 00	Formula IV (imbedded) 4th order
	2.000 000 000 36	Formula IV 5th order
	2.000 000 000 25	NYSTROM,
$n = 1$	2.000 000 000 13	Formula IV (imbedded) 4th order
	2.000 000 000 20	Formula IV 5th order
	2.000 000 001 33	NYSTROM,
$n = 2$	2.000 000 000 09	Formula IV (imbedded) 4th order
	2.000 000 000 10	Formula IV 5th order
	2.000 000 000 73	NYSTROM,
$n = 3$	2.000 000 000 05	Formula IV (imbedded) 4th order
	2.000 000 000 05	Formula IV 5th order
	2.000 000 000 38	NYSTROM,
$n = 4$	2.000 000 000 03	Formula IV (imbedded) 4th order
	2.000 000 000 03	Formula IV 5th order
	2.000 000 000 19	NYSTROM,
$n = 5$	2.000 000 000 01	Formula IV (imbedded) 4th order
	2.000 000 000 01	Formula IV 5th order
	2.000 000 000 10	NYSTROM,
$n = 6$	2.000 000 000 01	Formula IV (imbedded) 4th order
	2.000 000 000 01	Formula IV 5th order
	2.000 000 000 05	NYSTROM,
$n = 7$	2.000 000 000 00	Formula IV (imbedded) 4th order
	2.000 000 000 00	Formula IV 5th order
	2.000 000 000 02	NYSTROM,
$n = 8$	2.000 000 000 00	Formula IV (imbedded) 4th order
	2.000 000 000 00	Formula IV 5th order
	2.000 000 000 01	NYSTROM,
$n = 9$	2.000 000 000 00	Formula IV (imbedded) 4th order
	2.000 000 000 00	Formula IV 5th order
	2.000 000 000 01	NYSTROM,
$n = 10, \ldots, 15$	2.000 000 000 00	Same for all theree formulas.

In the following tables are listed the exact and approximate values for the solutions of the remaining two boundary value problems. When four values are listed consecutively in a box, the first, the second and the third represent approximations given by Formula IV (imbedded) fourth order, Formula IV fifth order and NYSTROM's formula, respectively; the last one represents the exact value obtained from the analytic solution $y = (x+1)^m$ $(m = 2, 5)$.

Problem: $\frac{dy}{dx} = \frac{2y}{x+1}$ with (0, 1).

$h = 2^{-n}$	Solutions	
$n = 0$	3.944 444 444 44	Formula IV (imbedded) 4th order
	3.983 333 334 55	Formula IV 5th order
	3.983 068 791 69	NYSTROM
	4.000 000 000 00	Exact value,
$n = 1$	2.246 666 666 67	Formula IV (imbedded) 4th order
	2.249 393 939 69	Formula IV 5th order
	2.249 385 867 45	NYSTROM
	2.250 000 000 00	Exact value,
$n = 2$	1.562 345 679 01	Formula IV (imbedded) 4th order
	1.562 484 253 03	Formula IV 5th order
	1.562 484 044 20	NYSTROM
	1.562 500 000 00	Exact value,
$n = 3$	1.265 618 992 70	Formula IV (imbedded) 4th order
	1.265 624 673 17	Formula IV 5th order
	1.265 624 668 65	NYSTROM
	1.265 625 000 00	Exact value,
$n = 4$	1.128 906 039 00	Formula IV (imbedded) 4th order
	1.128 906 244 07	Formula IV 5th order
	1.128 906 244 00	NYSTROM
	1.128 906 250 00	Exact value,
$n = 5$	1.063 476 555 50	Formula IV (imbedded) 4th order
	1.063 476 562 40	Formula IV 5th order
	1.063 476 562 40	NYSTROM
	1.063 476 562 50	Exact value,
$n = 6$	1.031 494 140 40	Formula IV (imbedded) 4th order
	1.031 494 140 62	Formula IV 5th order
	1.031 494 140 63	NYSTROM
	1.031 494 140 63	Exact value,
$n = 7$	1.015 686 035 15	Formula IV (imbedded) 4th order
	1.015 686 035 16	Formula IV 5th order
	1.015 686 035 16	NYSTROM
	1.015 686 035 16	Exact value,
$n = 8$	1.007 827 758 79	Same for all methods
$n = 9$	1.003 910 064 70	» » » »
$n = 10$	1.001 954 078 67	» » » »
$n = 11$	1.000 976 800 92	» » » »
$n = 12$	1.000 488 340 85	» » » »
$n = 13$	1.000 244 155 53	» » » »
$n = 14$	1.000 122 074 04	» » » »
$n = 15$	1.000 061 036 09	» » » » .

$h = 2^{-n}$	Approximations for $y(1) = 4$	
$n = 0$	3.94 444 444 444	Formula IV (imbedded) 4th order
	3.98 333 333 455	Formula IV 5th order
	3.98 306 879 169	NYSTROM,
$n = 1$	3.99 764 739 281	Formula IV (imbedded) 4th order
	3.99 875 591 863	Formula IV 5th order
	3.99 873 938 543	NYSTROM,
$n = 2$	3.99 990 725 784	Formula IV (imbedded) 4th order
	3.99 993 984 097	Formula IV 5th order
	3.99 993 903 766	NYSTROM,
$n = 3$	3.99 999 671 221	Formula IV (imbedded) 4th order
	3.99 999 769 798	Formula IV 5th order
	3.99 999 766 652	NYSTROM,
$n = 4$	3.99 999 989 081	Formula IV (imbedded) 4th order
	3.99 999 992 112	Formula IV 5th order
	3.99 999 992 062	NYSTROM,
$n = 5$	3.99 999 999 655	Formula IV (imbedded) 4th order
	3.99 999 999 749	Formula IV 5th order
	3.99 999 999 780	NYSTROM,
$n = 6$	3.99 999 999 992	Formula IV (imbedded) 4th order
	3.99 999 999 995	Formula IV 5th order
	4.00 000 000 013	NYSTROM,
$n = 7$	4.00 000 000 001	Formula IV (imbedded) 4th order
	4.00 000 000 002	Formula IV 5th order
	4.00 000 000 010	NYSTROM,
$n = 8$	4.00 000 000 001	Formula IV (imbedded) 4th order
	4.00 000 000 001	Formula IV 5th order
	4.00 000 000 005	NYSTROM,
$n = 9$	4.00 000 000 000	Formula IV (imbedded) 4th order
	4.00 000 000 000	Formula IV 5th order
	4.00 000 000 003	NYSTROM,
$n = 10$	4.00 000 000 000	Formula IV (imbedded) 4th order
	4.00 000 000 000	Formula IV 5th order
	4.00 000 000 001	NYSTROM,
$n = 11$	4.00 000 000 000	Formula IV (imbedded) 4th order
	4.00 000 000 000	Formula IV 5th order
	4.00 000 000 001	NYSTROM,
$n = 12, \ldots, 15$	4.00 000 000 000	Same for all formulas .

Problem: $\frac{dy}{dx} = \frac{5y}{x+1}$ with (0, 1).

$h = 2^{-n}$	Solutions	
$n = 0$	23.222 222 222 2	Formula IV (imbedded) 4th order
	24.916 666 676 1	Formula IV 5th order
	26.953 703 812 5	NYSTROM
	32.000 000 000 0	Exact value,
$n = 1$	7.166 666 666 67	Formula IV (imbedded) 4th order
	7.354 166 668 58	Formula IV 5th order
	7.436 779 588 27	NYSTROM
	7.593 750 000 00	Exact value,
$n = 2$	3.033 950 617 28	Formula IV (imbedded) 4th order
	3.045 697 909 17	Formula IV 5th order
	3.047 969 394 15	NYSTROM
	3.051 757 812 50	Exact value,
$n = 3$	1.801 374 471 36	Formula IV (imbedded) 4th order
	1.801 908 028 32	Formula IV 5th order
	1.801 956 531 58	NYSTROM
	1.802 032 470 70	Exact value,
$n = 4$	1.354 058 634 47	Formula IV (imbedded) 4th order
	1.354 078 903 03	Formula IV 5th order
	1.354 079 796 94	NYSTROM
	1.354 081 153 87	Exact value,
$n = 5$	1.166 324 861 04	Formula IV (imbedded) 4th order
	1.166 325 561 02	Formula IV 5th order
	1.166 325 576 24	NYSTROM
	1.166 325 598 96	Exact value,
$n = 6$	1.080 604 828 55	Formula IV (imbedded) 4th order
	1.080 604 851 56	Formula IV 5th order
	1.080 604 851 81	NYSTROM
	1.080 604 852 18	Exact value,
$n = 7$	1.039 677 637 84	Formula IV (imbedded) 4th order
	1.039 677 638 58	Formula IV 5th order
	1.039 677 638 59	NYSTROM
	1.039 677 638 59	Exact value,
$n = 8$	1.019 684 435 08	Formula IV (imbedded) 4th order
	1.019 684 435 10	Formula IV 5th order
	1.019 684 435 10	NYSTROM
	1.019 684 435 10	Exact value,
$n = 9$	1.009 803 846 55	Same for all methods
$n = 10$	1.004 892 358 56	» » » »
$n = 11$	1.002 443 791 60	» » » »
$n = 12$	1.001 221 299 32	» » » »
$n = 13$	1.000 610 500 59	» » » »
$n = 14$	1.000 305 213 04	» » » »
$n = 15$	1.000 152 597 20	» » » » .

$h = 2^{-n}$	Approximations for $y(1) = 32$	
$n = 0$	23.222 222 222 2	Formula IV (imbedded) 4th order
	24.916 666 676 1	Formula IV 5th order
	26.953 703 812 5	NYSTROM,
$n = 1$	30.492 276 085 0	Formula IV (imbedded) 4th order
	30.779 015 253 5	Formula IV 5th order
	31.202 752 235 5	NYSTROM,
$n = 2$	31.883 907 247 9	Formula IV (imbedded) 4th order
	31.900 023 779 6	Formula IV 5th order
	31.937 764 886 3	NYSTROM,
$n = 3$	31.994 241 153 7	Formula IV (imbedded) 4th order
	31.994 881 137 6	Formula IV 5th order
	31.996 885 320 2	NYSTROM,
$n = 4$	31.999 773 230 9	Formula IV (imbedded) 4th order
	31.999 795 557 5	Formula IV 5th order
	31.999 876 961 5	NYSTROM,
$n = 5$	31.999 992 052 5	Formula IV (imbedded) 4th order
	31.999 992 788 2	Formula IV 5th order
	31.999 995 690 6	NYSTROM,
$n = 6$	31.999 999 738 2	Formula IV (imbedded) 4th order
	31.999 999 761 8	Formula IV 5th order
	31.999 999 862 1	NYSTROM,
$n = 7$	31.999 999 992 2	Formula IV (imbedded) 4th order
	31.999 999 992 9	Formula IV 5th order
	31.999 999 998 0	NYSTROM,
$n = 8$	32.000 000 000 0	Formula IV (imbedded) 4th order
	32.000 000 000 1	Formula IV 5th order
	32.000 000 001 1	NYSTROM,
$n = 9$	32.000 000 000 2	Formula IV (imbedded) 4th order
	32.000 000 000 2	Formula IV 5th order
	32.000 000 000 6	NYSTROM,
$n = 10$	32.000 000 000 1	Formula IV (imbedded) 4th order
	32.000 000 000 1	Formula IV 5th order
	32.000 000 000 3	NYSTROM,
$n = 11$	32.000 000 000 0	Formula IV (imbedded) 4th order
	32.000 000 000 0	Formula IV 5th order
	32.000 000 000 2	NYSTROM,
$n = 12$	32.000 000 000 0	Formula IV (imbedded) 4th order
	32.000 000 000 0	Formula IV 5th order
	32.000 000 000 1	NYSTROM,
$n = 13$	32.000 000 000 0	Same for all formulas
$n = 14$	32.000 000 000 0	» » » »
$n = 15$	31.999 999 999 9	» » » » .

It is seen that when $n = 0, \ldots, 7$, i. e. with $h = 1$ through $h = 1/128$, the approximations provided by NYSTROM's formula to $y(1)$ are better than those of Formula IV. This is due to the following peculiar situation. In the considered problem these formulas provide approximations by defect. The rounding errors help to bring these approximations even closer to the true values. However, the rounding errors associated with NYSTROM's formula being larger than those associated with our formula, the former formula yields better results. In other words, in this instance the round-off errors constitute a useful asset rather than a liability.

However, with decreasing « h » , these errors decrease also so that starting with $n = 8$ up to $n = 12$ ($h = 1/256$ through $h = 1/8192$) the superiority of the Formula IV becomes once again apparent. The Formula IV provides the best possible results (in the considered problem and relative to the number of decimal figures retained) for $n = 11, 12, 13, 14$; NYSTROM's formula is equally good only for $n = 13, 14$.

As far as the accuracy of the obtained approximations is concerned, the preceding table shows that the application of our rule would indicate in the worst case ($h = 1/16$, $\tilde{y}_4 = 31.999\,773\,230\,9$, $\tilde{y}_5 = 31.999\,795\,557\,5$, $y(1) = 32.000\,000\,000\,0$) an error about 11 times smaller than the actual error. And these error estimates are obtained by the use of a simple internal property of pseudo-iterative formulas without recourse to evaluation of certain partial derivatives or other laborious processes [1] as presently are needed.

Furthermore as it will be seen in the next section, the pseudo-iterative formulas and the related error estimating efficient internal property can be extended with ease to systems of ordinary differential equations and to differential equations of higher order.

8. – Consider the systems of ordinary differential equations of the form

$$\frac{\mathrm{d}y^i}{\mathrm{d}x} = f^i(x, y^1, y^2, \ldots, y^s) \qquad (i = 1, \ldots, s) \tag{15}$$

subject to initial condition $y^i(x_0) = y^i_0$.

In order to extend the pseudo-iterative formulas and the related error estimating rule to (15) it suffices to regard (1) as a vector equation, the vectors being y and f [3]. It follows that the pseudo-iterative formulas associated with (1) must also be considered as vector formulas.

Then the vector equation (1), and associated pseudo-iterative vector formulas represent in compact form the system (15), and the set of pseudo-iterative formulas associated with the system, respectively.

Taking for instance $s = 2$ and for the sake of convenience letting $y^1 = y$ and $y^2 = z$, the system (15) can be written

$$(16)\qquad \begin{cases} \dfrac{dy}{dx} = f^1(x,\ y,\ z) \\[2ex] \dfrac{dz}{dx} = f^2(x,\ y,\ z) \end{cases}$$

with

$$y(x_0) = y_0\,, \qquad z(x_0) = z_0\,.$$

Regarding (1) as a vector equation representing in compact form (16), the pseudo-iterative vector Formula (IV) will then represent in compact form the following set of pseudo-iterative formulas corresponding to the system (16):

$$(17)\qquad \begin{cases} \tilde{y}_4(x_0 + h) = y_0 + \dfrac{1}{6}\,(k_0^1 + 4\,k_2^1 + k_3^1) \\[2ex] \tilde{z}_4(x_0 + h) = z_0 + \dfrac{1}{6}\,(k_0^2 + 4\,k_2^2 + k_3^2) \\[2ex] \tilde{y}_5(x_0 + h) = y_0 + \dfrac{1}{336}\,(14\,k_0^1 + 35\,k_3^1 + 162\,k_4^1 + 125\,k_5^1) \\[2ex] \tilde{z}_5(x_0 + h) = z_0 + \dfrac{1}{336}\,(14\,k_0^2 + 35\,k_3^2 + 162\,k_4^2 + 125\,k_5^2)\,, \end{cases}$$

where

$$\begin{cases} k_0^1 = h\,f^1(x_0\,,\ y_0\,,\ z_0) \\ k_0^2 = h\,f^2(x_0\,,\ y_0\,,\ z_0)\,, \end{cases}$$

$$\begin{cases} k_1^1 = h\,f^1\!\left(x_0 + \dfrac{1}{2}\,h\,,\quad y_0 + \dfrac{1}{2}\,k_0^1\,,\quad z_0 + \dfrac{1}{2}\,k_0^2\right) \\[2ex] k_1^2 = h\,f^2\!\left(x_0 + \dfrac{1}{2}\,h\,,\quad y_0 + \dfrac{1}{2}\,k_0^1\,,\quad z_0 + \dfrac{1}{2}\,k_0^2\right), \end{cases}$$

$$\begin{cases} k_2^1 = h\,f^1\!\left(x_0 + \dfrac{1}{2}\,h\,,\quad y_0 + \dfrac{1}{4}\,(k_0^1 + k_1^1)\,,\quad z_0 + \dfrac{1}{4}\,(k_0^2 + k_1^2)\right) \\[2ex] k_2^2 = h\,f^2\!\left(x_0 + \dfrac{1}{2}\,h\,,\quad y_0 + \dfrac{1}{4}\,(k_0^1 + k_1^1)\,,\quad z_0 + \dfrac{1}{4}\,(k_0^2 + k_1^2)\right), \end{cases}$$

$$\begin{cases} k_3^1 = h\, f^1(x_0 + h\,, \quad y_0 - k_1^1 + 2\, k_2^1\,, \quad z_0 - k_1^2 + 2\, k_2^2) \\ k_3^2 = h\, f^2(x_0 + h\,, \quad y_0 - k_1^1 + 2\, k_2^1\,, \quad z_0 - k_1^2 + 2\, k_2^2)\,, \end{cases}$$

$$\begin{cases} k_4^1 = h\, f^1\left(x_0 + \frac{2}{3}\,h, \quad y_0 + \frac{1}{27}\,(7\, k_0^1 + 10\, k_1^1 + k_3^1), \quad z_0 + \frac{1}{27}\,(7\, k_0^2 + 10\, k_1^2 + k_3^2)\right) \\ k_4^2 = h\, f^2\left(x_0 + \frac{2}{3}\,h, \quad y_0 + \frac{1}{27}\,(7\, k_0^1 + 10\, k_1^1 + k_3^1), \quad z_0 + \frac{1}{27}\,(7\, k_0^2 + 10\, k_1^2 + k_3^2)\right), \end{cases}$$

$$\begin{cases} k_5^1 = h\, f^1\Big(x_0 + \frac{2}{10}\,h, \quad y_0 + \frac{16}{10000}\,(28\, k_0^1 - 125\, k_1^1 + 546\, k_2^1 + 54\, k_3^1 - 378\, k_4^1), \\ \qquad\qquad z_0 + \frac{16}{10000}\,(28\, k_0^2 - 125\, k_1^2 + 546\, k_2^2 + 54\, k_3^2 - 378\, k_4^2)\Big) \\ k_5^2 = h\, f^2\Big(x_0 + \frac{2}{10}\,h, \quad y_0 + \frac{16}{10000}\,(28\, k_0^1 - 125\, k_1^1 + 546\, k_2^1 + 54\, k_3^1 - 378\, k_4^1), \\ \qquad\qquad z_0 + \frac{16}{10000}\,(28\, k_0^2 - 125\, k_1^2 + 546\, k_2^2 + 54 k_3^2 - 378\, k_4^2)\Big)\,. \end{cases}$$

The set of formulas (17) permit also the approximate solution of second order ordinary differential equations whether they are linear or not. Furthermore, they provide, again with almost no labor except that of taking the linear combination of a few k's already computed, error estimates which are as accurate as those obtained with any other method.

For an illustrative example let us consider the second order differential equation

$$(1 - x^2)\, y'' - 2\, x\, y' + 6\, y = 0 \tag{18}$$

subject to the initial conditions: $x = 0$, $y = -\frac{1}{2}$, $y' = 0$.

This is a LEGENDRE equation having as solution $y = (3x^2 - 1)/2$. We thus have also $y' = 3x$. The latter two polynomials permit for any x the determination of the corresponding exact values y and y'.

Letting $y' = z$ and consequently $y'' = z'$ the equation (18) is reduced to the system of first order differential equations:

$$\begin{cases} \dfrac{dy}{dx} = z \\ \dfrac{dz}{dx} = \dfrac{2xz - 6y}{1 - x^2} \end{cases}$$

with $x = 0$, $y = -\frac{1}{2}$, $z = 0$.

In the table below the first and second values listed in any box are the fourth and fifth order approximations obtained through the use of (17) while the third listing represents either one of the exact values y, y'.

$h = 0.1$	$\tilde{y}_4 =$	$-$ 0.484 999 811 711 410 7
	$\tilde{y}_5 =$	$-$ 0.485 000 630 384 442 2
	$y =$	$-$ 0.485 000 000 000 000 0
	$\tilde{y}'_4 =$	0.299 984 818 200 270 2
	$\tilde{y}'_5 =$	0.299 999 800 892 103 1
	$y' =$	0.300 000 000 000 000 0
$h = 0.05$	$\tilde{y}_4 =$	$-$ 0.496 249 997 088 064 7
	$\tilde{y}_5 =$	$-$ 0.496 250 009 817 248 6
	$y =$	$-$ 0.496 250 000 000 000 0
	$\tilde{y}'_4 =$	0.149 999 529 620 011 6
	$\tilde{y}'_5 =$	0.149 999 998 097 441 0
	$y' =$	0.150 000 000 000 000 0
$h = 0.025$	$\tilde{y}_4 =$	$-$ 0.499 062 499 966 627 6
	$\tilde{y}_5 =$	$-$ 0.499 062 500 162 385 5
	$y =$	$-$ 0.499 062 500 000 000 0
	$\tilde{y}'_4 =$	0.074 999 985 098 838 76
	$\tilde{y}'_5 =$	0.074 999 999 660 732 45
	$y' =$	0.075 000 000 000 000 00
$h = 0.0125$	$\tilde{y}_4 =$	$-$ 0.499 765 625 000 388 0
	$\tilde{y}_5 =$	$-$ 0.499 765 625 003 579 9
	$y =$	$-$ 0.499 765 625 000 000 0
	$\tilde{y}'_4 =$	0.037 499 999 379 118 27
	$\tilde{y}'_5 =$	0.037 499 999 791 561 13
	$y' =$	0.037 500 000 000 000 00
$h = 0.00625$	$\tilde{y}_4 =$	$-$ 0.499 941 406 250 339 5
	$\tilde{y}_5 =$	$-$ 0.499 941 406 250 504 6
	$y =$	$-$ 0.499 941 406 250 000 0
	$\tilde{y}'_4 =$	0.018 749 999 968 955 91
	$\tilde{y}'_5 =$	0.018 749 999 980 597 44
	$y' =$	0.018 750 000 000 000 00 .

When $h = 0.1$, apparently $\tilde{y}_4$ and $\tilde{y}_5$ have only 2 leading decimal figures in agreement. But since $|\tilde{y}_5 - \tilde{y}_4| = 0.000\,000\,8 < 10^{-6}$, we consider 10^{-6} as an upper bound for the committed absolute error in $\tilde{y}_5$ and accept the five leading decimal figures in $\tilde{y}_5$ as correct.

When $h = 0.05$, $\tilde{y}_4$ and $\tilde{y}_5$ have 4 leading decimal figures in agreement. But $|\tilde{y}_5 - \tilde{y}_4| \approx 10^{-8}$ and thus we accept the seven leading decimal figures in $\tilde{y}_5$ as correct.

When $h = 0.00625$ the application of the error estimating rule indicates that $\tilde{y}_5$ has its 12 leading decimal figures in agreement with the exact value.

On the other hand, when $h = 0.1$, 0.05, 0.025, 0.0125 and 0.00625 we find that $\tilde{y}'_5$ has apparently 4, 6, 7, 9 and 10 leading decimal figures in agreement with y', respectively.

All this information about the errors can be checked to be true.

We have equally good results even in the case of the repeated application of formula (17). For instance with $h = 0.00625$ after 16 applications of (17) we find at $x = 0.1$:

$$\begin{cases} \tilde{y}_4 = -0.485\,000\,000\,\underline{135}\,\underline{370\,0} \\ \tilde{y}_5 = -0.485\,000\,000\,\underline{146}\,\underline{803\,0} \end{cases} \quad \text{and} \quad \begin{cases} \tilde{y}'_4 = 0.299\,999\,998\,\underline{527}\,\underline{068\,8} \\ \tilde{y}'_5 = 0.299\,999\,998\,\underline{605}\,\underline{787\,8}\,. \end{cases}$$

The error estimating rule indicates that $\tilde{y}_5$ has 10 leading decimals in agreement with the exact value. Actually it has only 9 leading decimals in agreement. Furthermore, it indicates $0.000\,000\,000\,011$ to be the absolute error in $\tilde{y}_5$ instead of $0.000\,000\,000\,135$ which is about 12 times larger. For $\tilde{y}'_5$ the rule indicates 9 leading decimals in agreement with the exact value instead of 8 decimals.

Besides this, for the absolute error

$$|\tilde{y}'_5 - y'| = 0.000\,000\,001\,394 \qquad \text{it gives} \qquad 0.000\,000\,000\,078$$

which is 18 times smaller.

Before closing it is appropriate to quote from ([3], p. 109):

« Some authorities (Milne, Gill) recommend this reduction of equations of higher order to a system of equations of the first order also for numerical « purposes; others (Collatz) take the opposite position, arguing that reduction « to a first order system increases both the error and the necessary number of « operations. »

The results obtained through the use of pseudo-iterative formulas undoubtedly will bring more weight to the arguments of those who recommend the numerical solution of higher order differential equations be performed by first reducing them to a system of first order differential equations.

References.

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[6] D. SARAFYAN, *Error estimation for Runge-Kutta methods*, Notices Amer. Math. Soc. **12** (1965) (cf. p. 572).

[7] D. SARAFYAN, *Runge-Kutta formulas in pseudo-iterative form*, Notices Amer. Math. Soc. **13** (1966) (cf. p. 224).

[8] D. SARAFYAN, *Existence and approximation theorems for ordinary differential equations and their systems* (II), forthcoming.

Summary.

An internal error estimating property of Runge-Kutta formulas of any order is put into evidence. This property is easy to apply, but weak, and will be improved with the derivation of a new type of fifth order Runge-Kutta formulas exhibiting iterative properties, and for this reason referred to as pseudo-iterative Runge-Kutta formulas. These provide, by quantities that appear directly in the computation, 1st, 2nd, 4th and 5th order approximations. The comparison of these consecutively improved approximations readily yields valuable information about their accuracy, in particular, about that of the fifth order. The formulas and the method are simple, the approximations obtained, if not superior, are competitive with those provvided by known formulas.

* * *