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LOW-ORDER CLASSICAL RUNGE-KUTTA FORMULAS WITH STEPSIZE CONTROL AND THEIR APPLICATION TO SOME HEAT TRANSFER PROBLEMS

by Erwin Fehlberg

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INTRODUCTION

1. In an earlier report [1], the author derived fifth- to eighth-order RUNGE-KUTTA formulas with stepsize control. In this paper, similar first- to fourth-order formulas are developed.

2. Such low-order RUNGE-KUTTA formulas are of interest in some heat transfer problems. It is well-known that the parabolic partial differential equations of such problems can be reduced to ordinary differential equations. For instance, by a discretization of the space variable(s) of the problem, we obtain a system of ordinary differential equations with the time as the independent variable. Such a system can then be integrated by RUNGE-KUTTA methods.

3. However, it is also well-known that the application of RUNGE-KUTTA methods to such problems is often very time-consuming. Higher-order RUNGE-KUTTA formulas do not offer advantages in this respect, since stability considerations, resulting from the exponential character of the solution, exclude an increase of the integration stepsize that would make such high-order formulas meaningful. Therefore, low-order RUNGE-KUTTA formulas (second- or third-order) can be expected to solve such problems more efficiently than any high-order formula. On the other hand, they are potentially more efficient than the standard difference formulas obtained by discretization of the space variable(s) as well as the time variable.

4. For the efficiency of RUNGE-KUTTA formulas, it is essential that their truncation errors be as small as possible, since the permissable integration stepsize is strongly dependent upon the magnitude of these errors. Therefore, we have tried to establish RUNGE-KUTTA formulas with small truncation errors.

SECTION I. FOURTH-ORDER FORMULAS

5. We consider the (vector) differential equation

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

and write for our RUNGE-KUTTA formula ,

$$\left.\begin{aligned} f_o &= f(x_o, y_o) \\ f_\kappa &= f\left(x_o + \alpha_\kappa h,\ \sum_{\lambda=0}^{\kappa-1} \beta_{\kappa\lambda} f_\lambda\right) \quad (\kappa = 1, 2, 3, 4, 5) \end{aligned}\right\} \quad (2)$$

and

$$\left.\begin{aligned} y &= y_o + h \sum_{\kappa=0}^{4} c_\kappa f_\kappa + 0(h^5) \\ \hat{y} &= y_o + h \sum_{\kappa=0}^{5} \hat{c}_\kappa f_\kappa + 0(h^6) \end{aligned}\right\} \quad (3)$$

with h as integration stepsize and (x_o, y_o) as initial values. Equations (3) imply that we try to determine the coefficients α_κ, $\beta_{\kappa\lambda}$, c_κ, $\hat{c}_\kappa$ in such a way that the first formula (3) represents a fourth-order, and the second formula (3), a fifth-order RUNGE-KUTTA formula. The difference $y - \hat{y}$ then represents an approximation for the leading (fifth- order) truncation error term of our fourth-order RUNGE-KUTTA formula and can be used easily for establishing a reliable stepsize control procedure for this formula.

6. The coefficients α_κ, $\beta_{\kappa\lambda}$, c_κ, and $\hat{c}_\kappa$ have to satisfy certain equations of condition that can be obtained by TAYLOR expansions. These equations of condition are well-known in the literature, see for example J.C. BUTCHER's paper ([2], Table 1), or a paper by this author ([1], Table I). For the convenience of the reader, we list these equations here for a fifth-order formula like the second equation (3).

Introducing the abbreviations:

$$\left.\begin{aligned} &\beta_{\kappa 1}\alpha_1^\lambda + \beta_{\kappa 2}\alpha_2^\lambda \ldots\ldots + \beta_{\kappa\kappa-1}\alpha_{\kappa-1}^\lambda = P_{\kappa\lambda} \\ &(\kappa = 2, 3, 4, 5;\ \lambda = 1, 2, 3) \end{aligned}\right\} \quad (4)$$

Table I contains the 17 equations of condition for our fifth-order formula.

TABLE I. EQUATIONS OF CONDITION FOR FIFTH-ORDER FORMULA

$(\mathrm{I}, \hat{1})$ $$\sum_{\kappa=1}^{5} \hat{c}_\kappa - 1 = 0$$

$(\mathrm{II}, \hat{1})$ $$\sum_{\kappa=1}^{5} \hat{c}_\kappa \alpha_\kappa - \frac{1}{2} = 0$$

$(\mathrm{III}, \hat{1})$ $$\sum_{\kappa=2}^{5} \hat{c}_\kappa P_{\kappa 1} - \frac{1}{6} = 0$$

$(\mathrm{III}, \hat{2})$ $$\frac{1}{2} \sum_{\kappa=1}^{5} \hat{c}_\kappa \alpha_\kappa^2 - \frac{1}{6} = 0$$

$(\mathrm{IV}, \hat{1})$ $$\sum_{\kappa=3}^{5} \hat{c}_\kappa \left(\sum_{\lambda=2}^{\kappa-1} \beta_{\kappa\lambda} P_{\lambda 1} \right) - \frac{1}{24} = 0$$

$(\mathrm{IV}, \hat{2})$ $$\frac{1}{2} \sum_{\kappa=2}^{5} \hat{c}_\kappa P_{\kappa 2} - \frac{1}{24} = 0$$

$(\mathrm{IV}, \hat{3})$ $$\sum_{\kappa=2}^{5} \hat{c}_\kappa \alpha_\kappa P_{\kappa 1} - \frac{1}{8} = 0$$

$(\mathrm{IV}, \hat{4})$ $$\frac{1}{6} \sum_{\kappa=1}^{5} \hat{c}_\kappa \alpha_\kappa^3 - \frac{1}{24} = 0$$

$(\mathrm{V}, \hat{1})$ $$\sum_{\kappa=4}^{5} \hat{c}_\kappa \left[\sum_{\lambda=3}^{\kappa-1} \beta_{\kappa\lambda} \left(\sum_{\mu=2}^{\lambda-1} \beta_{\lambda\mu} P_{\mu 1} \right) \right] - \frac{1}{120} = 0$$

$(\mathrm{V}, \hat{2})$ $$\frac{1}{2} \sum_{\kappa=3}^{5} \hat{c}_\kappa \left(\sum_{\lambda=2}^{\kappa-1} \beta_{\kappa\lambda} P_{\lambda 2} \right) - \frac{1}{120} = 0$$

TABLE I. (Concluded)

$$(V,\hat{3})\qquad \sum_{\kappa=3}^{5} \hat{c}_\kappa \left(\sum_{\lambda=2}^{\kappa-1} \beta_{\kappa\lambda}\alpha_\lambda P_{\lambda 1} \right) - \frac{1}{40} = 0$$

$$(V,\hat{4})\qquad \frac{1}{6} \sum_{\kappa=2}^{5} \hat{c}_\kappa P_{\kappa 3} - \frac{1}{120} = 0$$

$$(V,\hat{5})\qquad \sum_{\kappa=3}^{5} \hat{c}_\kappa \alpha_\kappa \left(\sum_{\lambda=2}^{\kappa-1} \beta_{\kappa\lambda} P_{\lambda 1} \right) - \frac{1}{30} = 0$$

$$(V,\hat{6})\qquad \frac{1}{2} \sum_{\kappa=2}^{5} \hat{c}_\kappa \alpha_\kappa P_{\kappa 2} - \frac{1}{30} = 0$$

$$(V,\hat{7})\qquad \frac{1}{2} \sum_{\kappa=2}^{5} \hat{c}_\kappa P^2_{\kappa 1} - \frac{1}{40} = 0$$

$$(V,\hat{8})\qquad \frac{1}{2} \sum_{\kappa=2}^{5} \hat{c}_\kappa \alpha^2_\kappa P_{\kappa 1} - \frac{1}{20} = 0$$

$$(V,\hat{9})\qquad \frac{1}{24} \sum_{\kappa=1}^{5} \hat{c}_\kappa \alpha^4_\kappa - \frac{1}{120} = 0$$

The Roman numerals in front of the equations in Table I indicate the order of the terms in the TAYLOR expansion.

A similar table holds for a fourth-order formula such as the first formula (3). We obtain this table from Table I by omitting the fifth-order equations $(V,\hat{1})$ through $(V,\hat{9})$ and replacing, in the remaining equations, $\hat{c}_\kappa$ by c_κ and the upper limit 5 of the k-sums by 4. These remaining eight equations might be denoted by (I, 1) through (IV, 4).

All eight equations of this new table for a fourth-order formula and the 17 equations of Table I for a fifth-order formula have to be satisfied simultaneously.

7. For the following we assume

$$c_1 = 0, \qquad \hat{c}_1 = 0, \qquad \alpha_4 = 1 \tag{5}$$

We further assume that α_2, α_3, α_5 are different from one another and from 0 and 1.

Equations (II, 1), (III, 2), (IV, 4) then yield

$$\left.\begin{aligned}
c_2 &= \frac{1}{12}\,\frac{2\alpha_3 - 1}{\alpha_2(\alpha_3 - \alpha_2)(1 - \alpha_2)} \\
c_3 &= \frac{1}{12}\,\frac{2\alpha_2 - 1}{\alpha_3(\alpha_2 - \alpha_3)(1 - \alpha_3)} \\
c_4 &= \frac{1}{12}\,\frac{6\alpha_2\alpha_3 - 4(\alpha_2 + \alpha_3) + 3}{(1 - \alpha_2)(1 - \alpha_3)}
\end{aligned}\right\} \tag{6}$$

and equations $(\mathrm{II}, \hat{1})$, $(\mathrm{III}, \hat{2})$, $(\mathrm{IV}, \hat{4})$, $(\mathrm{V}, \hat{9})$

$$\left.\begin{aligned}
\hat{c}_2 &= \frac{1}{60}\,\frac{10\alpha_3\alpha_5 - 5(\alpha_3 + \alpha_5) + 3}{\alpha_2(\alpha_3 - \alpha_2)(1 - \alpha_2)(\alpha_5 - \alpha_2)} \\
\hat{c}_3 &= \frac{1}{60}\,\frac{10\alpha_2\alpha_5 - 5(\alpha_2 + \alpha_5) + 3}{\alpha_3(\alpha_2 - \alpha_3)(1 - \alpha_3)(\alpha_5 - \alpha_3)} \\
\hat{c}_4 &= \frac{1}{60}\,\frac{30\alpha_2\alpha_3\alpha_5 - 20(\alpha_2\alpha_3 + \alpha_2\alpha_5 + \alpha_3\alpha_5) + 15(\alpha_2 + \alpha_3 + \alpha_5) - 12}{(\alpha_2 - 1)(\alpha_3 - 1)(\alpha_5 - 1)} \\
\hat{c}_5 &= \frac{1}{60}\,\frac{10\alpha_2\alpha_3 - 5(\alpha_2 + \alpha_3) + 3}{\alpha_5(\alpha_2 - \alpha_5)(\alpha_3 - \alpha_5)(1 - \alpha_5)}
\end{aligned}\right\} \tag{7}$$

8. Furthermore, we make the following assumptions that greatly reduce the number of equations of condition

$$(A1)\begin{cases} P_{21} = \frac{1}{2}\alpha_2^2 \\ P_{31} = \frac{1}{2}\alpha_3^2 \\ P_{41} = \frac{1}{2} \\ P_{51} = \frac{1}{2}\alpha_5^2 \end{cases} \qquad (A2)\begin{cases} P_{22} = \frac{1}{3}\alpha_2^3 \\ P_{32} = \frac{1}{3}\alpha_3^3 \\ P_{42} = \frac{1}{3} \\ P_{52} = \frac{1}{3}\alpha_5^3 \end{cases}$$

$$(B) \qquad c_2\beta_{21} + c_3\beta_{31} + c_4\beta_{41} = 0$$

$$(\hat{B}) \qquad \hat{c}_2\beta_{21} + \hat{c}_3\beta_{31} + \hat{c}_4\beta_{41} + \hat{c}_5\beta_{51} = 0$$

$$(\hat{C}) \qquad \hat{c}_2\alpha_2\beta_{21} + \hat{c}_3\alpha_3\beta_{31} + \hat{c}_4\beta_{41} + \hat{c}_5\alpha_5\beta_{51} = 0$$

From (A1) and (A2) the following identities result:

$$\left.\begin{array}{l} (\mathrm{III},1) \equiv (\mathrm{III},2)\ ; \quad (\mathrm{IV},2) \equiv (\mathrm{IV},4)\ ; \quad (\mathrm{IV},3) \equiv 3(\mathrm{IV},4) \\ (\mathrm{III},\hat{1}) \equiv (\mathrm{III},\hat{2})\ ; \quad (\mathrm{IV},\hat{2}) \equiv (\mathrm{IV},\hat{4})\ ; \quad (\mathrm{IV},\hat{3}) \equiv 3(\mathrm{IV},4)\ ; \\ (\mathrm{V},\hat{6}) \equiv 4(\mathrm{V},\hat{9})\ ; \quad (\mathrm{V},\hat{7}) \equiv 3(\mathrm{V},\hat{9})\ ; \quad (\mathrm{V},\hat{8}) \equiv 6(\mathrm{V},\hat{9}) \end{array}\right\} \quad (8)$$

By also using (B) and $(\hat{B})$ we find the following identities:

$$\begin{array}{l} (\mathrm{IV},1) \equiv (\mathrm{IV},2) \\ (\mathrm{IV},\hat{1}) \equiv (\mathrm{IV},\hat{2})\ ; \quad (\mathrm{V},\hat{2}) \equiv (\mathrm{V},\hat{4})\ ; \quad (\mathrm{V},\hat{3}) \equiv 3(\mathrm{V},\hat{4}) \end{array} \qquad (9)$$

and finally by also taking into account assumption $(\hat{C})$

$$(\mathrm{V},\hat{5}) \equiv (\mathrm{V},\hat{6}) \qquad (10)$$

Therefore, equations (I, 1) ; $(\mathrm{I},\hat{1})$; $(\mathrm{V},\hat{1})$; $(\mathrm{V},\hat{4})$ are the only remaining equations of condition.

The first two equations determine the coefficients c_o and $\hat{c}_o$ that otherwise do not enter our equations of condition.

The remaining equations $(V, \hat{1})$ and $(V, \hat{4})$ have to be solved together with our assumptions (A1), (A2), (B), $(\hat{B})$, and $(\hat{C})$.

9. From the first equations (A1) and (A2), the following relations are obtained:

$$\alpha_1 = \frac{2}{3}\alpha_2 \tag{11}$$

$$\beta_{21} = \frac{3}{4}\alpha_2 \tag{12}$$

The second equations (A1) and (A2) yield

$$\left.\begin{aligned} \beta_{31} &= \frac{3}{4}\left(\frac{\alpha_3}{\alpha_2}\right)^2 (3\alpha_2 - 2\alpha_3) \\ \beta_{32} &= \left(\frac{\alpha_3}{\alpha_2}\right)^2 (\alpha_3 - \alpha_2) \end{aligned}\right\} \tag{13}$$

The third equations (A1) and (A2), together with (B), determine the coefficients β_{41}, β_{42}, β_{43}. We find the following expressions for these coefficients:

$$\left.\begin{aligned} \beta_{41} &= \frac{3}{4} \cdot \frac{1}{\alpha_2^2} \cdot \frac{6\alpha_2^2\alpha_3 - 6\alpha_2\alpha_3 + 2\alpha_3 - \alpha_2}{6\alpha_2\alpha_3 - 4(\alpha_2 + \alpha_3) + 3} \\ \beta_{42} &= -\frac{1}{\alpha_2^2} \cdot \frac{1 - \alpha_2}{\alpha_3 - \alpha_2} \cdot \frac{2\alpha_2^2\alpha_3 - 4\alpha_2\alpha_3 + \alpha_3^2 + \alpha_2}{6\alpha_2\alpha_3 - 4(\alpha_2 + \alpha_3) + 3} \\ \beta_{43} &= -\frac{1}{\alpha_3} \cdot \frac{(1 - \alpha_2)(1 - \alpha_3)}{\alpha_3 - \alpha_2} \cdot \frac{2\alpha_2 - 1}{6\alpha_2\alpha_3 - 4(\alpha_2 + \alpha_3) + 3} \end{aligned}\right\} \tag{14}$$

Elimination of $\hat{c}_5$ from $(\hat{B})$ and $(\hat{C})$ leads to the following relation:

$$\hat{c}_2(\alpha_5 - \alpha_2)\beta_{21} + \hat{c}_3(\alpha_5 - \alpha_3)\beta_{31} + \hat{c}_4(\alpha_5 - 1)\beta_{41} = 0 \tag{15}$$

Introducing the above computed values for $\hat{c}_2$, $\hat{c}_3$, $\hat{c}_4$, β_{21}, β_{31}, and β_{41} into (15) leads to a relation between α_2, α_3, and α_5.

$$M\alpha_5 = N \tag{16}$$

with

$$\left.\begin{aligned} M = {} & (6\alpha_2\alpha_3 - 4\alpha_2 - 4\alpha_3 + 3)\,(30\alpha_2\alpha_3^2 - 30\alpha_2^2\alpha_3^2 - 10\alpha_3^2 + 5\alpha_2\alpha_3) \\ & + (6\alpha_2^2\alpha_3 - 6\alpha_2\alpha_3 + 2\alpha_3 - \alpha_2)(30\alpha_2\alpha_3^2 - 20\alpha_2\alpha_3 - 20\alpha_3^2 + 15\alpha_3) \\ N = {} & (6\alpha_2\alpha_3 - 4\alpha_2 - 4\alpha_3 + 3)\,(16\alpha_2\alpha_3^2 - 15\alpha_2^2\alpha_3^2 - 6\alpha_3^2 + 3\alpha_2\alpha_3) \\ & + (6\alpha_2^2\alpha_3 - 6\alpha_2\alpha_3 + 2\alpha_3 - \alpha_2)\,(20\alpha_2\alpha_3^2 - 15\alpha_2\alpha_3 - 15\alpha_3^2 + 12\alpha_3) \end{aligned}\right\} \quad (17)$$

It is easily verified that

$$M = 0 \tag{18}$$

for any value of α_2 and α_3 .

Because of (16), only such values as α_2 and α_3 are possible that also lead to

$$N = 0 \tag{19}$$

Equation (19) represents a restrictive relation between α_2 and α_3. This relation can be reduced to

$$\alpha_3 = \frac{1}{2} \cdot \frac{\alpha_2}{5\alpha^2 - 4\alpha_2 + 1} \tag{20}$$

10. We use relation (20) to eliminate α_3 from the expressions for our RUNGE-KUTTA coefficients as obtained in Nos. 7, 8, and 9. The elimination results in

$$\left.\begin{aligned} \alpha_1 &= \frac{2}{3}\alpha_2 \\ \alpha_3 &= \frac{1}{2} \cdot \frac{\alpha_2}{5\alpha_2^2 - 4\alpha_2 + 1} \\ c_2 &= \frac{1}{6} \cdot \frac{1}{\alpha_2^2(1 - \alpha_2)} \cdot \frac{5\alpha_2^2 - 5\alpha_2 + 1}{10\alpha_2^2 - 8\alpha_2 + 1} \end{aligned}\right\} \quad (21)$$

$$
\left.
\begin{aligned}
c_3 &= \frac{2}{3} \cdot \frac{1}{\alpha_2^2 (5\alpha_2 - 2)} \cdot \frac{(5\alpha_2^2 - 4\alpha_2 + 1)^3}{10\alpha_2^2 - 8\alpha_2 + 1} \\
c_4 &= \frac{1}{6} \cdot \frac{10\alpha_2^2 - 12\alpha_2 + 3}{(1 - \alpha_2)(5\alpha_2 - 2)} \\
\beta_{21} &= \frac{3}{4}\alpha_2 \\
\beta_{31} &= \frac{3}{16}\alpha_2 \cdot \frac{15\alpha_2^2 - 12\alpha_2 + 2}{(5\alpha_2^2 - 4\alpha_2 + 1)^3} \\
\beta_{32} &= -\frac{1}{8}\alpha_2 \cdot \frac{10\alpha_2^2 - 8\alpha_2 + 1}{(5\alpha_2^2 - 4\alpha_2 + 1)^3} \\
\beta_{41} &= \frac{3}{4} \cdot \frac{1}{10\alpha_2^2 - 12\alpha_2 + 3} \\
\beta_{42} &= -\frac{1}{2} \cdot \frac{1 - \alpha_2}{\alpha_2^2} \cdot \frac{60\alpha_2^3 - 78\alpha_2^2 + 31\alpha_2 - 4}{(10\alpha_2^2 - 12\alpha_2 + 3)(10\alpha_2^2 - 8\alpha_2 + 1)} \\
\beta_{43} &= -2 \cdot \frac{(1 - \alpha_2)(5\alpha_2 - 2)(2\alpha_2 - 1)(5\alpha_2^2 - 4\alpha_2 + 1)^2}{\alpha_2^2(10\alpha_2^2 - 12\alpha_2 + 3)(10\alpha_2^2 - 8\alpha_2 + 1)}
\end{aligned}
\right\} \quad \begin{matrix}(21) \\ \text{(continued)}\end{matrix}
$$

11. The weight factors $\hat{c}_2$ through $\hat{c}_5$ of the fifth-order formula can now be expressed by α_2 and α_5:

$$
\left.
\begin{aligned}
\hat{c}_2 &= \frac{1}{60} \cdot \frac{10\alpha_5(5\alpha_2^2 - 5\alpha_2 + 1) - (30\alpha_2^2 - 29\alpha_2 + 6)}{\alpha_2^2(10\alpha_2^2 - 8\alpha_2 + 1)(1 - \alpha_2)(\alpha_5 - \alpha_2)} \\
\hat{c}_3 &= \frac{4}{15} \cdot \frac{(5\alpha_2^2 - 4\alpha_2 + 1)^4 [5\alpha_5(2\alpha_2 - 1) - (5\alpha_2 - 3)]}{\alpha_2^2(10\alpha_2^2 - 8\alpha_2 + 1)(5\alpha_2^2 - 2)(2\alpha_2 - 1)[2\alpha_5(5\alpha_2^2 - 4\alpha_2 + 1) - \alpha_2]} \\
\hat{c}_4 &= \frac{1}{60} \cdot \frac{10(2\alpha_2 - 1)(10\alpha_2^2 - 12\alpha_2 + 3)\alpha_5 - (150\alpha_2^3 - 260\alpha_2^2 + 141\alpha_2 - 24)}{(1 - \alpha_2)(5\alpha_2 - 2)(2\alpha_2 - 1)(1 - \alpha_5)} \\
\hat{c}_5 &= \frac{1}{60} \cdot \frac{(5\alpha_2 - 2)(10\alpha_2^2 - 12\alpha_2 + 3)}{\alpha_5(1 - \alpha_5)(\alpha_2 - \alpha_5)[2(5\alpha_2^2 - 4\alpha_2 + 1)\alpha_5 - \alpha_2]}
\end{aligned}
\right\} (22)
$$

12. We still have to determine the coefficients β_{51}, β_{52}, β_{53}, β_{54} of our fifth-order formula. From equation (B) we find β_{51}. The fourth equations (A1) and (A2) together with equation $(V, \hat{4})$, determine the coefficients β_{52}, β_{53}, β_{54}. It can be shown that equation $(V, \hat{1})$ is then also satisfied for any value of α_2 and α_5.

This concludes the computation of our RUNGE-KUTTA coefficients, since c_o and $\hat{c}_o$ can be determined from (I, 1) or $(I, \hat{1})$, respectively, and the coefficients $\beta_{\kappa o}$ $(\kappa = 1, 2, 3, 4, 5)$ can be obtained from the standard equations

$$\sum_{\lambda=0}^{\kappa-1} \beta_{\kappa\lambda} = \alpha_\kappa \qquad (\kappa = 1, 2, 3, 4, 5) \tag{23}$$

13. Our RUNGE-KUTTA coefficients contain two arbitrary parameters, α_2 and α_5. We shall show that we can reduce the truncation error of our fourth-order formula by a proper choice of the parameter α_2. From Table I, it follows that the leading term (the fifth-order term) of the truncation error consists of nine sub-terms. These sub-terms are certain expressions built up by the partial derivatives of the right-hand sides of the differential equation (1). These sub-terms are multiplied by certain numerical factors T_1 through T_9. For these factors, we find from equations $V, \hat{1})$ through $(V, \hat{9})$ of Table I, replacing $\hat{c}_\kappa$ by c_κ and the upper limit 5 of the κ-sums by 4,

$$\left.\begin{aligned}
T_1 &= c_4\beta_{43}\beta_{32}P_{21} - \frac{1}{120} \\
T_2 &= \frac{1}{2}\sum_{\kappa=3}^{4} c_\kappa \left(\sum_{\lambda=2}^{\kappa-1} \beta_{\kappa\lambda} P_{\lambda 2} \right) - \frac{1}{120} \\
&\;\;\vdots \\
T_9 &= \frac{1}{24}\sum_{\kappa=1}^{4} c_\kappa \alpha_\kappa^4 - \frac{1}{120}
\end{aligned}\right\} \tag{24}$$

Naturally, it is desirable to find RUNGE-KUTTA formulas with small numerical factors T_1 through T_9 to make the leading term of the local truncation error small.

14. Since we can express all RUNGE-KUTTA coefficients that enter the right-hand sides of (24) by α_2 alone, the factors $T_1, \ldots, T_9$ can finally be written as functions of α_2. The computation results in the following values for these factors:

$$\left.\begin{aligned} T_1 = -T_5 &= -\frac{1}{240}\,\frac{(5\alpha_2 - 2)\,(4\alpha_2 - 1)}{5\alpha_2^2 - 4\alpha_2 + 1} \\ T_2 = \frac{1}{3}T_3 = T_4 = -T_6 &= -\frac{4}{3}T_7 = -\frac{2}{3}T_8 = 4T_9 \\ &= \frac{1}{720}\,\frac{(5\alpha_2 - 2)\,(10\alpha_2^2 - 12\alpha_2 + 3)}{5\alpha_2^2 - 4\alpha_2 + 1} \end{aligned}\right\} \tag{25}$$

15. We see from (25) that all factors $T_1, \ldots, T_9$ would become zero for $\alpha_2 = \frac{2}{5}$. Because of (20), this value α_2 leads to $\alpha_3 = 1$. It can, however, be shown easily that $\alpha_3 = \alpha_4 = 1$ leads to contradictions in the equations (II, 1), (III, 2), (IV, 4) and $(\text{II}, \hat{1})$, $(\text{III}, \hat{2})$, $(\text{IV}, \hat{4})$, $(\text{V}, \hat{9})$. Therefore, we have to exclude the value $\alpha_2 = \frac{2}{5}$.

Another interesting choice of α_2 would result from

$$10\alpha_2^2 - 12\alpha_2 + 3 = 0 \tag{26}$$

If (26) would hold, all error factors in the second group of (25) would become zero.

Because of (26), it would follow from (21),

$$c_4 = 0 \tag{27}$$

It can be shown easily that for the values α_2 resulting from (26) and for $c_4 = 0$, equation (B) cannot be satisfied.

Therefore, we also have to discard the values $\alpha_2 = \frac{1}{10}(6 \pm \sqrt{6}) \approx \begin{cases} 0.845 \\ 0.355 \end{cases}$ resulting from (26).

However, by choosing for α_2 a value close to one of the above values, say close to 0.355, we can expect that at least the error factors in the second group of (25) will become small.

We shall consider two choices for α_2 that are reasonably close to 0.355 and lead to relatively simple RUNGE-KUTTA coefficients, namely $\alpha_2 = \frac{1}{3}$ and $\alpha_2 = \frac{3}{8}$. The choice of α_5 in our formulas remains arbitrary.

16. Choosing $\alpha_2 = \frac{1}{3}$ leads to the RUNGE-KUTTA coefficients of Table II.

TABLE II. COEFFICIENTS FOR RK4(5), FORMULA 1

$\kappa \backslash \lambda$	α_κ	$\beta_{k\lambda}$ 0	1	2	3	4	c_κ	$\hat{c}_\kappa$
0	0	0					$\frac{1}{9}$	$\frac{47}{450}$
1	$\frac{2}{9}$	$\frac{2}{9}$					0	0
2	$\frac{1}{3}$	$\frac{1}{12}$	$\frac{1}{4}$				$\frac{9}{20}$	$\frac{12}{25}$
3	$\frac{3}{4}$	$\frac{69}{128}$	$-\frac{243}{128}$	$\frac{135}{64}$			$\frac{16}{45}$	$\frac{32}{225}$
4	1	$-\frac{17}{12}$	$\frac{27}{4}$	$-\frac{27}{5}$	$\frac{16}{15}$		$\frac{1}{12}$	$\frac{1}{30}$
5	$\frac{5}{6}$	$\frac{65}{432}$	$-\frac{5}{16}$	$\frac{13}{16}$	$\frac{4}{27}$	$\frac{5}{144}$		$\frac{6}{25}$

Subtracting the last two columns of Table II from one another, one finds as approximation for the leading term of the local truncation error of our fourth-order formula

$$TE = \left(\frac{1}{150} f_o - \frac{3}{100} f_2 + \frac{16}{75} f_3 + \frac{1}{20} f_4 - \frac{6}{25} f_5\right) h \tag{28}$$

We also list the error factors T_1 through T_9 of our formula 1:

$$\left.\begin{aligned} &T_1 = \frac{1}{480}, \quad T_2 = -\frac{1}{4320}, \quad T_3 = -\frac{1}{1440}, \quad T_4 = -\frac{1}{4320}, \\ &T_5 = -\frac{1}{480}, \quad T_6 = \frac{1}{4320}, \quad T_7 = \frac{1}{5760}, \quad T_8 = \frac{1}{2880}, \\ &T_9 = \frac{1}{17280} \end{aligned}\right\} \tag{29}$$

17. For our second choice, $\alpha_2 = \frac{3}{8}$, we find the RUNGE-KUTTA coefficients of Table III.

TABLE III. COEFFICIENTS FOR RK4(5), FORMULA 2

$\kappa \backslash \lambda$	α_κ	$\beta_{\kappa\lambda}$ 0	1	2	3	4	c_κ	$\hat{c}_\kappa$
0	0	0					$\frac{25}{216}$	$\frac{16}{135}$
1	$\frac{1}{4}$	$\frac{1}{4}$					0	0
2	$\frac{3}{8}$	$\frac{3}{32}$	$\frac{9}{32}$				$\frac{1408}{2565}$	$\frac{6656}{12825}$
3	$\frac{12}{13}$	$\frac{1932}{2197}$	$-\frac{7200}{2197}$	$\frac{7296}{2197}$			$\frac{2197}{4104}$	$\frac{28561}{56430}$
4	1	$\frac{439}{216}$	-8	$\frac{3680}{513}$	$-\frac{845}{4104}$		$-\frac{1}{5}$	$-\frac{9}{50}$
5	$\frac{1}{2}$	$-\frac{8}{27}$	2	$-\frac{3544}{2565}$	$\frac{1859}{4104}$	$-\frac{11}{40}$		$\frac{2}{55}$

For the leading term of the local truncation error we obtain from Table III the approximation

$$TE = \left(-\frac{1}{360} f_o + \frac{128}{4275} f_2 + \frac{2187}{75240} f_3 - \frac{1}{50} f_4 - \frac{2}{55} f_5 \right) h \quad (30)$$

This formula 2 has the following error factors:

$$\left.\begin{aligned} & T_1 = \frac{1}{780}, \quad T_2 = \frac{1}{12480}, \quad T_3 = \frac{1}{4160}, \quad T_4 = \frac{1}{12480}, \\ & T_5 = -\frac{1}{780}, \quad T_6 = -\frac{1}{12480}, \quad T_7 = -\frac{1}{16640}, \\ & T_8 = -\frac{1}{8320}, \quad T_9 = -\frac{1}{49920} \end{aligned}\right\} \quad (31)$$

We notice that the error factors (31) of our second formula are somewhat smaller than the corresponding terms (29) of our first formula.

18. We should like to mention that another RK4(5)-formula was derived by D. SARAFYAN ([3], p. 4). His fourth-order formula is based upon only four (instead of five) evaluations of the differential equations. Therefore, his fourth-order formula has larger error terms than our formulas.

Since SARAFYAN's formula is published in an internal Technical Report and therefore is not easily accessible, we present SARAFYAN's formula as Table IV.

From Table IV it follows for the leading term of the local truncation error

$$TE = \left(\frac{1}{8} f_o + \frac{2}{3} f_2 + \frac{1}{16} f_3 - \frac{27}{56} f_4 - \frac{125}{336} f_5 \right) h \quad (32)$$

The error factors T_1 through T_9 for SARAFYAN's formula read as follows:

$$\left.\begin{aligned} & T_1 = -\frac{1}{120}, \quad T_2 = \frac{1}{480}, \quad T_3 = -\frac{1}{240}, \quad T_4 = -\frac{1}{720}, \\ & T_5 = \frac{1}{120}, \quad T_6 = -\frac{1}{480}, \quad T_7 = \frac{1}{960}, \quad T_8 = \frac{1}{480}, \\ & T_9 = \frac{1}{2880} \end{aligned}\right\} \quad (33)$$

TABLE IV. COEFFICIENTS FOR SARAFYAN'S RK4(5)-FORMULA

κ \ λ	α_κ	$\beta_{\kappa\lambda}$ 0	1	2	3	4	c_κ	$\hat{c}_\kappa$
0	0	0					$\frac{1}{6}$	$\frac{1}{24}$
1	$\frac{1}{2}$	$\frac{1}{2}$					0	0
2	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{4}$				$\frac{2}{3}$	0
3	1	0	-1	2			$\frac{1}{6}$	$\frac{5}{48}$
4	$\frac{2}{3}$	$\frac{7}{27}$	$\frac{10}{27}$	0	$\frac{1}{27}$			$\frac{27}{56}$
5	$\frac{1}{5}$	$\frac{28}{625}$	$-\frac{1}{5}$	$\frac{546}{625}$	$\frac{54}{625}$	$-\frac{378}{625}$		$\frac{125}{336}$

If we compare (33) with (31), we notice that in (31) the factors T_1 and T_5 are only $\frac{2}{13}$ of the corresponding factors of (33); the other factors of (31) are even smaller compared with the corresponding factors of (33).

For our RK4(5)-formula number 1, the error factors are $\frac{1}{4}$ (or better) of the corresponding error factors of SARAFYAN.

Because of the smaller error factors we may expect that our RK4(5) formulas 1 and 2 operate somewhat more economically than SARAFYAN's formula. Numerical experiments on an electronic computer have confirmed these expectations.

19. It is interesting to compare the error factors of SARAFYAN's formula with those of KUTTA's ([4], p. 443) standard fourth-order formula of Table V.

TABLE V. COEFFICIENTS FOR KUTTA'S RK4-FORMULA

κ \ λ	α_κ	$\beta_{\kappa\lambda}$ 0	$\beta_{\kappa\lambda}$ 1	$\beta_{\kappa\lambda}$ 2	c_κ
0	0	0			$\frac{1}{6}$
1	$\frac{1}{2}$	$\frac{1}{2}$			$\frac{1}{3}$
2	$\frac{1}{2}$	0	$\frac{1}{2}$		$\frac{1}{3}$
3	1	0	0	1	$\frac{1}{6}$

The computation shows that KUTTA's error factors are identical with the error factors (33) of SARAFYAN, except for T_7, which in the case of KUTTA's formulas has to be replaced by $\frac{1}{160}$.

Therefore, SARAFYAN's formula, in general, will not reduce substantially the number of integration steps required by KUTTA's formula. However, it will reduce the computer time, since it requires only six evaluations per step compared to seven in KUTTA's formula, if the latter one is applied with the standard stepsize control procedure (recomputation of two steps as one step with double stepsize).

20. We might mention that we have presented general RUNGE-KUTTA transformation formulas with stepsize control in two earlier papers [5], [6]. In the special case of a fourth-order formula these general formulas do not require any differentiation and can also be written in the form of classical RUNGE-KUTTA formulas.

SECTION II. THIRD-ORDER FORMULAS

21. Since a fourth-order RUNGE-KUTTA formula requires four evaluations (per step) of the differential equations, one might expect a pair of RUNGE-KUTTA formulas RK3(4) to require four evaluations also.

However, it can be shown easily that four evaluations are not sufficient to define the pair RK3(4). The equations of condition lead to contradictions in the case of four evaluations. We therefore allow for five evaluations per step.

However, it is possible to choose the fifth evaluation in such a way that this evaluation can be taken over as the first evaluation for the next step. Thereby the number of evaluations per step again will be reduced to four, except for the very first step, when the integration is started.

Since the derivation of the RK3(4)-formulas is very similar to the derivation of the RK4(5)-formulas of Section I, we may omit some details and present the main results only.

22. The equations of condition, as they hold for a fourth-order formula, are listed in Table VI.

TABLE VI. EQUATIONS OF CONDITION FOR FOURTH-ORDER FORMULA

$$(\mathrm{I}, \hat{1}) \qquad \sum_{\kappa=0}^{4} \hat{c}_\kappa - 1 = 0$$

$$(\mathrm{II}, \hat{1}) \qquad \sum_{\kappa=1}^{4} \hat{c}_\kappa \alpha_\kappa - \frac{1}{2} = 0$$

$$(\mathrm{III}, \hat{1}) \qquad \sum_{\kappa=2}^{4} \hat{c}_\kappa P_{\kappa 1} - \frac{1}{6} = 0$$

$$(\mathrm{III}, \hat{2}) \qquad \frac{1}{2} \sum_{\kappa=1}^{4} \hat{c}_\kappa \alpha_\kappa^2 - \frac{1}{6} = 0$$

$$(\mathrm{IV}, \hat{1}) \qquad \sum_{\kappa=3}^{4} \hat{c}_\kappa \left(\sum_{\lambda=2}^{\kappa-1} \beta_{\kappa\lambda} P_{\lambda 1} \right) - \frac{1}{24} = 0$$

$$(\mathrm{IV}, \hat{2}) \qquad \frac{1}{2} \sum_{\kappa=2}^{4} \hat{c}_\kappa P_{\kappa 2} - \frac{1}{24} = 0$$

TABLE VI. (Concluded)

$$(\mathrm{IV}, \hat{3}) \quad \sum_{\kappa=2}^{4} \hat{c}_\kappa \alpha_\kappa P_{\kappa 1} - \frac{1}{8} = 0$$

$$(\mathrm{IV}, \hat{4}) \quad \frac{1}{6} \cdot \sum_{\kappa=1}^{4} \hat{c}_\kappa \alpha_\kappa^3 - \frac{1}{24} = 0$$

A similar table for a third-order formula is obtained from Table VI by omitting the fourth-order equations of condition and replacing, in the remaining equations, $\hat{c}_\kappa$ by c_κ and the upper limit 4 of the κ-sums by 3.

We denote the remaining four equations for the third-order RUNGE-KUTTA formula by (I, 1), (II, 1), (III, 1), and (III, 2).

23. Again assuming that the conditions (5) hold and that α_2, α_3 are different from one another and from 0 and 1, we find from (II, 1) and (III, 2):

$$\left.\begin{aligned} c_2 &= \frac{1}{6} \cdot \frac{3\alpha_3 - 2}{\alpha_2(\alpha_3 - \alpha_2)} \\ c_3 &= \frac{1}{6} \cdot \frac{3\alpha_2 - 2}{\alpha_3(\alpha_2 - \alpha_3)} \end{aligned}\right\} \tag{34}$$

and from $(\mathrm{II}, \hat{1})$, $(\mathrm{III}, \hat{2})$, $(\mathrm{IV}, \hat{4})$:

$$\left.\begin{aligned} \hat{c}_2 &= \frac{1}{12} \cdot \frac{2\alpha_3 - 1}{\alpha_2(\alpha_3 - \alpha_2)(1 - \alpha_2)} \\ \hat{c}_3 &= \frac{1}{12} \cdot \frac{2\alpha_2 - 1}{\alpha_3(\alpha_2 - \alpha_3)(1 - \alpha_3)} \\ \hat{c}_4 &= \frac{1}{12} \cdot \frac{6\alpha_2\alpha_3 - 4(\alpha_2 + \alpha_3) + 3}{(1 - \alpha_2)(1 - \alpha_3)} \end{aligned}\right\} \tag{35}$$

24. To bring the remaining equations of condition into a form that can be handled more easily, we make, similar to Section I, the further assumptions

$$
(A) \quad \begin{cases} P_{21} = \frac{1}{2}\alpha_2^2 \\ P_{31} = \frac{1}{2}\alpha_3^2 \\ P_{41} = \frac{1}{2} \end{cases}
$$

$$
(\hat{B}) \qquad \hat{c}_2\beta_{21} + \hat{c}_3\beta_{31} + \hat{c}_4\beta_{41} = 0
$$

$$
(\hat{D}) \qquad \beta_{40} = c_0, \quad \beta_{41} = c_1 = 0, \quad \beta_{42} = c_2, \quad \beta_{43} = c_3
$$

The assumption $(\hat{D})$ is required if the fifth evaluation is to be taken over as the first evaluation for the next step.

From the assumptions (A), $(\hat{B})$, $(\hat{D})$, it follows immediately that the remaining equations of condition reduce to

$$
\left.\begin{array}{ll}
(IV, \hat{2}) & \hat{c}_3\beta_{32}\alpha_2^2 + \hat{c}_4 \cdot \frac{1}{3} = \frac{1}{12} \\[2ex]
(A) & \begin{cases} \beta_{21}\alpha_1 = \frac{1}{2}\alpha_2^2 \\ \beta_{31}\alpha_1 + \beta_{32}\alpha_2 = \frac{1}{2}\alpha_3^2 \end{cases} \\[2ex]
(\hat{B}) & \hat{c}_2\beta_{21} + \hat{c}_3\beta_{31} = 0
\end{array}\right\} \qquad (36)
$$

25. The first equation (A) expresses $\beta_{21}\alpha_1$ by α_2. From equation $(IV, \hat{2})$ we obtain β_{32} as a function of α_2 and α_3, since $\hat{c}_3$ and $\hat{c}_4$ are given as functions of α_2 and α_3 by (35).

The second equation (A) can then serve to find $\beta_{31}\alpha_1$ as function of α_2 and α_3.

The equation $(\hat{B})$, finally, represents a restrictive condition that must hold between α_2 and α_3 to make the equations of condition compatible. The computation results in the following restrictive condition:

$$\alpha_3 = \frac{1}{2} \cdot \frac{\alpha_2}{3\alpha_2^2 - 3\alpha_2 + 1} \qquad (37)$$

Eliminating α_3 from the coefficients of our third-order formula, these coefficients become functions of α_2 only. We find the following expressions for them:

$$\left.\begin{aligned}
c_2 &= \frac{1}{6} \cdot \frac{1}{\alpha_2^2} \cdot \frac{12\alpha_2^2 - 15\alpha_2 + 4}{6\alpha_2^2 - 6\alpha_2 + 1} \\
c_3 &= \frac{2}{3} \cdot \frac{1}{\alpha_2^2} \frac{(3\alpha_2 - 2)(3\alpha_2^2 - 3\alpha_2 + 1)^2}{6\alpha_2^2 - 6\alpha_2 + 1} \\
\beta_{21}\alpha_1 &= \frac{1}{2}\alpha_2^2 \\
\beta_{31}\alpha_1 &= \frac{1}{8}\alpha_2^2 \frac{(3\alpha_2 - 1)(3\alpha_2 - 2)}{(3\alpha_2^2 - 3\alpha_2 + 1)^3} \\
\beta_{32} &= -\frac{1}{8}\alpha_2 \frac{6\alpha_2^2 - 6\alpha_2 + 1}{(3\alpha_2^2 - 3\alpha_2 + 1)^3}
\end{aligned}\right\} \qquad (38)$$

26. We now consider the error factors for our third-order formula and try to make these error factors small by a proper choice of α_2 .

From Table V we find the following four error factors:

$$\left.\begin{aligned}
T_1 &= c_3\beta_{32} P_{21} - \frac{1}{24} \\
T_2 &= \frac{1}{2}(c_2 P_{22} + c_3 P_{32}) - \frac{1}{24} \\
T_3 &= c_2\alpha_2 P_{21} + c_3\alpha_3 P_{31} - \frac{1}{8} \\
T_4 &= \frac{1}{6}(c_2\alpha_2^3 + c_3\alpha_3^3) - \frac{1}{24}
\end{aligned}\right\} \qquad (39)$$

or, if we insert (38) into (39):

$$\left.\begin{aligned}
T_1 &= -\frac{1}{24}\,\frac{(2\alpha_2 - 1)(3\alpha_2 - 1)}{3\alpha_2^2 - 3\alpha_2 + 1} \\
T_2 &= \frac{1}{8}\,\alpha_1 \cdot \frac{\alpha_2(2\alpha_2 - 1)}{3\alpha_2^2 - 3\alpha_2 + 1} - \frac{1}{24}\,\frac{(3\alpha_2 - 1)(2\alpha_2 - 1)}{3\alpha_2^2 - 3\alpha_2 + 1} \\
T_3 &= \frac{1}{8}\,\frac{(\alpha_2 - 1)(2\alpha_2 - 1)^2}{3\alpha_2^2 - 3\alpha_2 + 1} \\
T_4 &= \frac{1}{24}\,\frac{(\alpha_2 - 1)(2\alpha_2 - 1)^2}{3\alpha_2^2 - 3\alpha_2 + 1}
\end{aligned}\right\} \qquad (40)$$

From the second equation (40), it follows that we can make $T_2 = 0$ by choosing

$$\alpha_1 = \frac{3\alpha_2 - 1}{3\alpha_2} \qquad (41)$$

27. All four error factors would become zero for $\alpha_2 = \frac{1}{2}$. This means for this choice of α_2, our third-order formula would actually become a fourth-order formula. Our pair RK3(4) of RUNGE-KUTTA formulas of the third- and of the fourth-order would degenerate into one fourth-order formula.

However, by choosing for α_2 a value close to $\frac{1}{2}$, we obtain RK3(4)-formulas with small error factors (40). We give two examples for such formulas with small error factors.

28. Choosing $\alpha_2 = \frac{4}{9}$, we obtain the RUNGE-KUTTA coefficients of Table VII.

For the leading term of the local truncation error we find from Table VII

$$TE = \left(\frac{5}{288} f_o - \frac{27}{416} f_2 + \frac{245}{1872} f_3 - \frac{1}{12} f_4\right) h \qquad (42)$$

For the four error factors of the formula of Table VII we obtain

$$T_1 = \frac{1}{168}, \quad T_2 = 0, \quad T_3 = -\frac{5}{1512}, \quad T_4 = -\frac{5}{4536} \qquad (43)$$

TABLE VII. COEFFICIENTS FOR RK3(4), FORMULA 1

κ \ λ	α_κ	$\beta_{\kappa\lambda}$ 0	1	2	3	c_κ	$\hat{c}_\kappa$
0	0	0				$\frac{1}{6}$	$\frac{43}{288}$
1	$\frac{1}{4}$	$\frac{1}{4}$				0	0
2	$\frac{4}{9}$	$\frac{4}{81}$	$\frac{32}{81}$			$\frac{27}{52}$	$\frac{243}{416}$
3	$\frac{6}{7}$	$\frac{57}{98}$	$-\frac{432}{343}$	$\frac{1053}{686}$		$\frac{49}{156}$	$\frac{343}{1872}$
4	1	$\frac{1}{6}$	0	$\frac{27}{52}$	$\frac{49}{156}$		$\frac{1}{12}$

29. Another suitable choice for α_2 would be $\alpha_2 = \frac{7}{15}$. For this value of α_2 we list the RUNGE-KUTTA coefficients in Table VIII.

TABLE VIII. COEFFICIENTS FOR RK3(4), FORMULA 2

κ \ λ	α_κ	$\beta_{\kappa\lambda}$ 0	1	2	3	c_κ	$\hat{c}_\kappa$
0	0	0				$\frac{79}{490}$	$\frac{229}{1470}$
1	$\frac{2}{7}$	$\frac{2}{7}$				0	0
2	$\frac{7}{15}$	$\frac{77}{900}$	$\frac{343}{900}$			$\frac{2175}{3626}$	$\frac{1125}{1813}$
3	$\frac{35}{38}$	$\frac{805}{1444}$	$-\frac{77175}{54872}$	$\frac{97125}{54872}$		$\frac{2166}{9065}$	$\frac{13718}{81585}$
4	1	$\frac{79}{490}$	0	$\frac{2175}{3626}$	$\frac{2166}{9065}$		$\frac{1}{18}$

For the formula of Table VIII we obtain

$$TE = \left(\frac{4}{735} f_o - \frac{75}{3626} f_2 + \frac{5776}{81585} f_3 - \frac{1}{18} f_4 \right) h \tag{44}$$

and the four error factors

$$T_1 = \frac{1}{228}, \quad T_2 = 0 , \quad T_3 - \frac{1}{855} , \quad T_4 = - \frac{1}{2565} \tag{45}$$

30. For comparison, we list KUTTA's third-order formula ([4], p. 440) in Table IX. His formula reads:

TABLE IX. COEFFICIENTS FOR KUTTA'S RK3-FORMULA

$\kappa \backslash \lambda$	α_κ	$\beta_{\kappa\lambda}$		c_κ
		0	1	
0	0	0		$\frac{1}{6}$
1	$\frac{1}{2}$	$\frac{1}{2}$		$\frac{2}{3}$
2	1	-1	2	$\frac{1}{6}$

It has the following error factors:

$$T_1 = - \frac{1}{24} , \quad T_2 = 0 , \quad T_3 = \frac{1}{24}, \quad T_4 = 0 \tag{46}$$

Comparing (43) and (45) with (46), we see that the largest value of (43) is only $\frac{1}{7}$ and the largest value of (45) only $\frac{2}{19}$ of the largest value of (46).

Therefore, our formulas of Table VII and Table VIII can be expected to be more economical than KUTTA's RK3-formula.

Since KUTTA's formula does not provide for a stepsize control, it requires five evaluations per step if operated with the standard stepsize procedure (recomputation of two steps as one step with double stepsize).

SECTION III. SECOND-ORDER FORMULAS

31. Allowing for four evaluations per step for an RK2(3)-formula, we list in Table X the equations of condition for a third-order formula.

TABLE X. EQUATIONS OF CONDITION FOR THIRD-ORDER FORMULA

$(\mathrm{I}, \hat{1})$ $$\sum_{\kappa=0}^{3} \hat{c}_\kappa - 1 = 0$$

$(\mathrm{II}, \hat{1})$ $$\sum_{\kappa=1}^{3} \hat{c}_\kappa \alpha_\kappa - \frac{1}{2} = 0$$

$(\mathrm{III}, \hat{1})$ $$\sum_{\kappa=2}^{3} \hat{c}_\kappa P_{\kappa 1} - \frac{1}{6} = 0$$

$(\mathrm{III}, \hat{2})$ $$\frac{1}{2} \sum_{\kappa=1}^{3} \hat{c}_\kappa \alpha_\kappa^2 - \frac{1}{6} = 0$$

32. We want to use the fourth evaluation of the differential equations as the first evaluation for the next step. This requires the conditions

$$\alpha_3 = 1 , \quad \beta_{30} = c_0 , \quad \beta_{31} = c_1 , \quad \beta_{32} = c_2 \tag{47}$$

where the c_ν's are the weight factors of the second-order formula, which is obtained from the first two equations of Table IX, replacing $\hat{c}_\nu$ by c_ν and the upper index 3 of κ-sums by 2. We denote those equations for the second-order formula by (I, 1) and (II, 1).

Furthermore, we assume

$$\hat{c}_1 = 0 \tag{48}$$

and

$$(A) \quad \left\{ \begin{aligned} P_{21} &= \frac{1}{2}\alpha_2^2 \\ P_{31} &= \frac{1}{2} \end{aligned} \right.$$

33. Because of (A), equations $(\mathrm{III}, \hat{1})$ and $(\mathrm{III}, \hat{2})$ become identical. Therefore, we can omit equation $(\mathrm{III}, \hat{1})$ from Table X.

From equations $(\mathrm{II}, \hat{1})$ and $(\mathrm{III}, \hat{2})$ we obtain, because of $\hat{c}_1 = 0$ and $\alpha_3 = 1$,

$$\left. \begin{aligned} \hat{c}_2 &= \frac{1}{6} \cdot \frac{1}{\alpha_2(1 - \alpha_2)} \\ \hat{c}_3 &= \frac{1}{6} \cdot \frac{2 - 3\alpha_2}{1 - \alpha_2} \end{aligned} \right\} \tag{49}$$

34. Let us now consider the error factors of our second-order formula. From the last two equations of Table X, we obtain for the two error factors the expressions

$$\left. \begin{aligned} T_1 &= c_2 \beta_{21} \alpha_1 - \frac{1}{6} \\ T_2 &= \frac{1}{2}(c_1\alpha_1^2 + c_2\alpha_2^2) - \frac{1}{6} \end{aligned} \right\} \tag{50}$$

Because of the first equation (A), we can write for the first equation (50),

$$T_1 = \frac{1}{2} c_2\alpha_2^2 - \frac{1}{6} = T_2 - \frac{1}{2} c_1\alpha_1^2 \tag{51}$$

or,

$$T_2 - T_1 = \frac{1}{2} c_1\alpha_1^2 \tag{52}$$

From (52), it follows that $T_2 \neq T_1$, assuming $c_1 \neq 0$.

For the following, we might assume

$$T_2 = -T_1 \tag{53}$$

By a proper choice of α_1 and α_2 we try to make T_1 and $T_2 = -T_1$ sufficiently small.

From (51), (52), and (53) we find

$$T_1 = \frac{1}{2} c_2\alpha_2^2 - \frac{1}{6} = -\frac{1}{4} c_1\alpha_1^2$$

or

$$c_1\alpha_1^2 + 2c_2\alpha_2^2 = \frac{2}{3} \tag{54}$$

Equation (54) and equation (II, 2) represent a system of two linear equations for c_1 and c_2.

The system has the solution

$$\left.\begin{aligned} c_1 &= \frac{1}{3} \cdot \frac{2 - 3\alpha_2}{\alpha_1(\alpha_1 - 2\alpha_2)} \\ c_2 &= \frac{1}{6} \cdot \frac{3\alpha_1 - 4}{\alpha_2(\alpha_1 - 2\alpha_2)} \end{aligned}\right\} \tag{55}$$

Introducing the expression (55) for c_2 into (51) yields

$$T_1 = \frac{1}{12} \alpha_1 \frac{3\alpha_2 - 2}{\alpha_1 - 2\alpha_2} \tag{56}$$

35. From equation (56), it follows that we could make $T_1 = T_2 = 0$ by choosing $\alpha_2 = \frac{2}{3}$. However, as in the case of our third-order formula RK3(4), our pair of RUNGE-KUTTA formulas RK2(3) would then degenerate into a single third-order formula.

However, by choosing α_2 close to $\frac{2}{3}$, we might obtain a suitable pair of RK2(3)-formulas with small error factors T_1 and T_2.

Choosing $\alpha_2 = \frac{27}{40}$ and $\alpha_1 = \frac{1}{4}$, we find the RUNGE-KUTTA coefficients of Table XI as follows.

TABLE XI. COEFFICIENTS FOR RK2(3)

$\kappa \backslash \lambda$	α_κ	$\beta_{\kappa\lambda}$ 0	1	2	c_κ	$\hat{c}_\kappa$
0	0	0			$\frac{214}{891}$	$\frac{533}{2106}$
1	$\frac{1}{4}$	$\frac{1}{4}$			$\frac{1}{33}$	0
2	$\frac{27}{40}$	$-\frac{189}{800}$	$\frac{729}{800}$		$\frac{650}{891}$	$\frac{800}{1053}$
3	1	$\frac{214}{891}$	$\frac{1}{33}$	$\frac{650}{891}$		$-\frac{1}{78}$

From Table XI we find for the leading term of the local truncation error the approximation

$$TE = \left(- \frac{23}{1782} f_0 + \frac{1}{33} f_1 - \frac{350}{11583} f_2 + \frac{1}{78} f_3 \right) h \tag{57}$$

The error factors for our RK2(3)-formula would read

$$T_1 = - \frac{1}{2112}, \quad T_2 = + \frac{1}{2112} \tag{58}$$

36. It is well-known that second-order RUNGE-KUTTA formulas RK2 can be obtained by two evaluations only. It is also possible to provide a stepsize control procedure by a third evaluation. We list in Table XII an example for such a RK2(3)-formula.

For the truncation error we find from Table XII the approximation

$$TE = \left(\frac{1}{3} f_0 + \frac{1}{3} f_1 - \frac{2}{3} f_2 \right) h \tag{59}$$

TABLE XII. COEFFICIENTS FOR RK2(3), BASED ON THREE EVALUATIONS

$\kappa \backslash \lambda$	α_κ	$\beta_{\kappa\lambda}$ 0	$\beta_{\kappa\lambda}$ 1	c_κ	$\hat{c}_\kappa$
0	0	0		$\frac{1}{2}$	$\frac{1}{6}$
1	1	1		$\frac{1}{2}$	$\frac{1}{6}$
2	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{4}$		$\frac{2}{3}$

The error factors for the formula of Table XII would read

$$T_1 = -\frac{1}{6}, \quad T_2 = \frac{1}{12} \tag{60}$$

It is interesting to note that KUTTA's third-order formula (Table IX) can also be operated as a second-order formula RK2(3) with stepsize control. We have to change only the weight factors of the formula, considering the c_κ-values of Table IX as $\hat{c}_\kappa$-values of the RK2(3)-formula and using $c_0 = 0$ $c_1 = 1$ as its c_κ-values.

Comparing (58) with (60), we notice that the error factors of our formula of Table XI are only $\frac{1}{352}$ of the larger error factor (60). Therefore, we may again expect our formula of Table XI to be more economical than the formula of Table XII, since the formula of Table XI also requires only three evaluations per step (except for the very first integration step).

SECTION IV. FIRST-ORDER FORMULA

37. If we base our RUNGE-KUTTA formula RK1(2) upon three evaluations per step, we obtain for the second-order formula the following equations of condition.

TABLE XIII. EQUATIONS OF CONDITION FOR SECOND-ORDER FORMULA

$(\mathrm{I}, \hat{1})$ $\quad \sum_{\kappa=0}^{2} \hat{c}_\kappa - 1 = 0$

$(\mathrm{II}, \hat{1})$ $\quad \sum_{\kappa=1}^{2} \hat{c}_\kappa \alpha_\kappa - \frac{1}{2} = 0$

Since we intend to use the third evaluation again as the first evaluation for the next step, we require

$$\alpha_2 = 1, \quad \beta_{20} = c_0, \quad \beta_{21} = c_1 \tag{61}$$

where c_0 and c_1 are the weight factors of the first-order formula, which is obtained from the first equation of Table XIII, replacing $\hat{c}_\nu$ by c_ν and the upper index 2 of the κ-sum by 1. Let us denote this equation for the first-order formula by $(\mathrm{I}, 1)$.

Obviously, there is only one error factor T_1, obtained from $(\mathrm{II}, \hat{1})$ as:

$$T_1 = c_1 \alpha_1 - \frac{1}{2} \tag{62}$$

We have to make this error factor small to obtain an efficient RK1(2)-formula. However, we should not make T_1 zero, since our pair of formulas RK1(2) would degenerate for $T_1 = 0$ into one second-order formula. We choose as coefficients the values of Table XIV:

TABLE XIV. COEFFICIENTS FOR RK1(2)

$\kappa \backslash \lambda$	α_κ	$\beta_{\kappa\lambda}$: 0	$\beta_{\kappa\lambda}$: 1	c_κ	$\hat{c}_\kappa$
0	0			$\frac{1}{256}$	$\frac{1}{512}$
1	$\frac{1}{2}$	$\frac{1}{2}$		$\frac{255}{256}$	$\frac{255}{256}$
2	1	$\frac{1}{256}$	$\frac{255}{256}$		$\frac{1}{512}$

which clearly satisfy equations $(\mathrm{I}, 1)$, $(\mathrm{I}, \hat{1})$, and $(\mathrm{II}, \hat{1})$.

For the approximate truncation error we find

$$TE = \frac{1}{512}(f_0 - f_2)\,h, \tag{63}$$

and the error factor T_1 becomes

$$T_1 = -\frac{1}{512} \tag{64}$$

38. EULER-CAUCHY's method can be considered as a first-order RUNGE-KUTTA formula, requiring only one evaluation per step. The method can even be operated as a RUNGE-KUTTA formula RK1(2) without additional evaluations by adding a second evaluation that can again be taken over as the first evaluation for the next step.

The resulting pair of formulas is shown in Table XV.

TABLE XV. EULER-CAUCHY'S METHOD AS RK1(2)

κ \ λ	α_κ	$\beta_{\kappa\lambda}$: 0	c_κ	$\hat{c}_\kappa$
0	0		1	$\frac{1}{2}$
1	1	1		$\frac{1}{2}$

The second-order formula RK2 of Table XV is obviously the so-called modified EULER-CAUCHY method.

Table XV yields as approximate truncation error

$$TE = \frac{1}{2}(f_0 - f_1)\,h \tag{65}$$

The error factor for the RK1(2)-formula of Table XV becomes

$$T_1 = -\frac{1}{2} \tag{66}$$

Comparison of (64) and (66) clearly shows that our formula of Table XIV will be more efficient than the formula of Table XV. Even the one additional evaluation per step required by our formula of Table XIV, in general, will not outweigh the advantage of the much smaller error factor.

We shall present a numerical example in Section V.

SECTION V. A NUMERICAL EXAMPLE (ORDINARY DIFFERENTIAL EQUATIONS)

39. In this section we present the numerical results of our new formulas for the same example that we considered in our earlier NASA report ([1], p. 30):

$$\left.\begin{array}{l} y' = -2xy \cdot \log z, \quad z' = 2xz \cdot \log y \\ \text{Initial values:} \quad x_0 = 0, \quad y_0 = e, \quad z_0 = 1 \\ \text{Exact solution:} \quad y = e^{\cos(x^2)}, \quad z = e^{\sin(x^2)} \end{array}\right\} \tag{67}$$

For reasons of comparison, we also include the results for some formulas of other authors. Our results are presented in Table XVI, the results of our new formulas being marked by an asterisk (*).

The numerical integration of problem (67) was executed on an IBM-7094 computer. All methods listed in Table XVI were run in single precision (eight decimal digits) and with the same tolerance (10^{-8}) for the local truncation error. Since the first-order formulas require a very small stepsize, we ran these formulas only up to $x = 5$; for the higher-order formulas the integration was performed up to $x = 25$.

40. Table XVI shows that the small error factors of our new formulas (*) make themselves felt in a considerable reduction of the number of integration steps and, therefore, of the computer time required for our problem.

The greatest reduction gained was for our first- and second-order formulas. For these formulas we required only about $\frac{1}{9}$ and about $\frac{1}{6}$ of the computer time of the corresponding conventional formulas. In the case of the third-order formula, we could cut the computer time to less than $\frac{1}{2}$, compared

TABLE XVI. COMPARISON OF THE VARIOUS METHODS FOR EXAMPLE (67)

	Method	Order of Method	Number of Evaluations Per Step	x_{max}	Number of Steps	Total Number of Evaluations	Running Time (min) on IBM-7094	Accumulated Errors in y and z: Δy	Δz
					Results for $x = x_{max}$ (Tolerance: 10^{-8})				
	EULER-CAUCHY (Table XV)	1	1	5	269 956	269 956	2.90	$+0.3018 \cdot 10^{-2}$	$-0.2945 \cdot 10^{-3}$
(*)	RK1(2) (Table XIV)	1	2	5	16 871	33 742	0.32	$+0.1926 \cdot 10^{-3}$	$-0.1543 \cdot 10^{-4}$
	RK2(3) (Table XII)	2	3	25	243 510	730 530	6.43	$+0.1458 \cdot 10^{-4}$	$-0.1781 \cdot 10^{-3}$
(*)	RK2(3) (Table XI)	2	3	25	37 493	112 479	1.13	$-0.1874 \cdot 10^{-4}$	$-0.8330 \cdot 10^{-5}$
	KUTTA (Table IX)	3	5	25	41 862	209 310	1.91	$+0.2190 \cdot 10^{-5}$	$-0.4664 \cdot 10^{-5}$
(*)	RK3(4) (Table VII)	3	4	25	23 225	92 900	0.90	$-0.2611 \cdot 10^{-5}$	$+0.1639 \cdot 10^{-4}$
(*)	RK3(4) (Table VIII)	3	4	25	22 054	88 216	0.85	$-0.2578 \cdot 10^{-5}$	$+0.1474 \cdot 10^{-4}$
	KUTTA (Table V)	4	7	25	16 010	112 070	0.95	$+0.1881 \cdot 10^{-5}$	$+0.2207 \cdot 10^{-4}$
	SARAFYAN (Table IV)	4	6	25	14 746	88 476	0.81	$-0.1546 \cdot 10^{-5}$	$-0.2086 \cdot 10^{-6}$
(*)	RK4(5) (Table II)	4	6	25	11 059	66 354	0.68	$+0.1222 \cdot 10^{-5}$	$+0.2015 \cdot 10^{-4}$
(*)	RK4(5) (Table III)	4	6	25	9 947	59 682	0.58	$+0.2041 \cdot 10^{-5}$	$+0.2512 \cdot 10^{-4}$

with KUTTA's formula. For fourth-order formulas our gains are more modest. Out second fourth-order formula (Table III), however, still requires only about $\frac{3}{5}$ of the computer time of KUTTA's formula and about $\frac{3}{4}$ of the time of SARAFYAN's formula.

The accuracy of our new formulas is about the same as that of the conventional formulas, except for the case of the first-order formulas. In this case we gain one more decimal digit with our new formula. Because the number of steps required by our new formula is only about $\frac{1}{16}$ of the number of steps of EULER-CAUCHY's formula, we do not accumulate round-off errors as heavily as the latter formula.

Compared with the conventional RUNGE-KUTTA formulas our new formulas offer results of the same accuracy in a fraction of the computer time. Therefore, our new formulas might be of interest for the numerical integration of ordinary differential equations.

Moreover, we shall show in the following sections of this paper that they can also be applied successfully to certain partial differential equations of the parabolic type.

SECTION VI. APPLICATION TO HEAT TRANSFER PROBLEMS

41. Let us consider the one-dimensional heat transfer problem

$$\left.\begin{array}{l} \dfrac{\partial u}{\partial t} = \dfrac{\partial^2 u}{\partial x^2} \\ \text{Initial Condition:} \quad t = 0 : u(x, 0) = u_0(x) \\ \text{Boundary Conditions:} \left\{\begin{array}{l} x = 0 : u(0, t) = b_0(t) \\ x = 1 : u(1, t) = b_1(t) \end{array}\right. \end{array}\right\} \qquad (68)$$

The first equation of (68) represents the simplest partial differential equation of the parabolic type.

Problem (68) requires finding a quantity u (usually the temperature) as function of the space variable x and the time variable t.

The existence of a solution of the problem (68) can be shown, under proper assumptions, by Fourier series methods. See, for example, the textbook by CARSLAW and JAEGER ([7], pp. 76-88). A quite elementary proof of the uniqueness of the solution of (68) is given in a textbook by BIEBERBACH ([8], pp. 352-353).

42. Replacing both derivatives of the first equation (68) by finite differences, one obtains the well-known difference equation

$$\frac{u_{i,j+1} - u_{i,j}}{k} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} \tag{69}$$

with $k = \Delta t$ and $h = \Delta x$.

Equation (69) is widely used for obtaining numerical solutions of problem (68), since this is the simplest explicit approach to the problem.

In applying (69) one has to pay attention to the fact that the mesh sizes h and k have to satisfy the well-known stability condition

$$r = \frac{k}{h^2} \leqq \frac{1}{2} \tag{70}$$

The condition (70) represents a certain restriction for the time mesh k if the space mesh h is given.

To preserve a reasonable accuracy of the results one has to apply a small space mesh h. In some problems the time mesh k, resulting from (70), may then become prohibitively small.

Furthermore, one has to consider that the mesh size k, resulting from (70), will guarantee the stability of the results, but no estimate of the local truncation error can be obtained from (70).

43. There exist other difference methods without stability restrictions, for example, the explicit method of DU FORT-FRANKEL [9]:

$$\frac{u_{i,j+1} - u_{i,j-1}}{2k} = \frac{u_{i+1,j} - (u_{i,j+1} + u_{i,j-1}) + u_{i-1,j}}{h^2}, \quad (71)$$

or the implicit method of CRANK-NICOLSON [10]:

$$\frac{u_{i,j+1} - u_{i,j}}{k} = \frac{1}{2}\left\{\frac{u_{i+1,j+1} - 2u_{i,j+1} + u_{i-1,j+1}}{h^2} + \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2}\right\} \quad (72)$$

However, other difficulties occur in the application of these two methods. The method of DU FORT-FRANKEL is a three-level method (time levels j-1, j, j+1) requiring a special starting procedure and additional considerations for a stepsize change of the time step. In the case of the implicit method of CRANK-NICOLSON, one has to solve a system of linear equations of the triple-diagonal form for each time step.

Although these difficulties might not be considered too serious, these methods again do not furnish an estimate of the local truncation error. Since they have no stability restrictions, an increased danger exists in that the integration could be performed with too large a time step. If this is the case, one would lose any accuracy, and, after a certain number of time steps, the computed u-values would bear little resemblence to the solution of the problem.

Equations (72) and (69) have identical left-hand sides; they approximate the time derivative $\frac{\partial u}{\partial t}$ by the same first-order accurate, finite difference. Therefore, the time integration of the CRANK-NICOLSON method cannot be more accurate than in the case of the explicit method (69).

44. If one wants to take full advantage of the accuracy that modern electronic computers are capable of, a more accurate approximation of the partial derivatives in the heat transfer equation — first equation (68) — and a current stepsize control for the integration become absolute necessities. A convenient way to achieve these objectives consists of converting the heat transfer equation into a system of ordinary differential equations by replacing the space derivative only by a finite difference. The resulting system of ordinary differential equations can then be integrated by RUNGE-KUTTA methods.

This is not a new procedure; it was suggested long ago by D. R. HARTREE and collaborators ([11] and [12], p. 254). They suggest replacing the first equation (68) by the system

$$\frac{du_i(\tau)}{d\tau} = u_{i+1}(\tau) - 2u_i(\tau) + u_{i-1}(\tau) = \delta^2 u_i(\tau) \tag{73}$$

with $\tau = \frac{t}{h^2}$.

Naturally, one can apply a better approximation to $\frac{\partial^2 u}{\partial x^2}$ by using higher-order central differences, resulting in

$$\frac{du_i(\tau)}{d\tau} = \delta^2 u_i(\tau) - \frac{1}{12}\delta^4 u_i(\tau) + \frac{1}{90}\delta^6 u_i(\tau) - + \dots \tag{74}$$

Formula (74) is suggested in GOODWIN's book ([13], p. 113).

In equations (73) and (74) the authors used the standard fourth-order RUNGE-KUTTA formula (Table V) for the numerical integration. GOODWIN ([13], pp. 114-115) and FOX ([14], pp. 240-241) point out that the fourth-order RUNGE-KUTTA method offers few advantages compared with the explicit difference formula (69), since the stability restriction of the RUNGE-KUTTA method is only slightly better ($r < 0.7$ instead of $r < 0.5$). On the other hand, the RUNGE-KUTTA method requires considerably more computer time per time step than formula (69). Therefore, it might seem questionable whether RUNGE-KUTTA methods are really worthwhile for application to problems such as (68).

45. We feel that the explicit difference method (69) certainly has its merits when applied to the computationally simple problem (68) and when requiring a moderate accuracy only.

However, the new low-order RUNGE-KUTTA formulas with stepsize control that are presented in this paper show the application of RUNGE-KUTTA formulas to parabolic partial differential equations in a different light, especially in connection with the use of highly accurate electronic computers.

For our numerical computations we used an eight-decimal digit computer (IBM-7094), and, when applying our new RUNGE-KUTTA formulas to heat transfer problems, we required that the local truncation error became negligible. This means we required that the local truncation error not contribute to the eight leading digits that the computer carries.

By doing so, we were able, when using higher-order central differences for the space derivatives, to obtain by means of our new RUNGE-KUTTA formulas, five to six good digits, even after a considerable number of integration steps. (See the examples in Section VII.) We found that these somewhat severe accuracy requirements could be well-satisfied by our low-order RUNGE-KUTTA methods and that we did not run into stability problems with these low-order methods since our accuracy requirements are much sharper than the stability requirements of our formulas.

46. Comparing the explicit difference method (69) with EULER-CAUCHY's method (Table XV), we see that both methods are identical as far as the time integration is concerned. Since the method of Table XV yields a convenient stepsize control procedure we have substituted EULER-CAUCHY's method of Table XV, for the explicit difference method (69).

47. Naturally, the explicit difference method and any RUNGE-KUTTA method can be run in a fraction of the computer time if we apply less severe accuracy restrictions, for example, if we apply the stability restriction only. However, such a relaxation of the accuracy restriction would result in a severe loss of accuracy.

48. The RUNGE-KUTTA methods are not restricted to the simple problem (68). They can be applied to more involved one-dimensional heat transfer problems, as outlined in the next section. Multi-dimensional heat transfer problems can also be made amenable to RUNGE-KUTTA methods when replacing all space derivatives by proper finite differences.

SECTION VII. TWO NUMERICAL EXAMPLES (HEAT TRANSFER PROBLEMS)

49. In this section we present numerical results of our new RUNGE-KUTTA formulas for two one-dimensional heat transfer problems. In both problems the exact solution is available so that the errors of our formulas can be stated.

First problem:

$$\left.\begin{array}{l}
\dfrac{\partial u}{\partial t} = \dfrac{1}{4} \cdot \dfrac{e^2}{2 + x^2} \cdot e^{-u} \cdot \dfrac{\partial^2 u}{\partial x^2} \\[2ex]
\text{Initial Condition:} \quad t = 0 : u = 2\left[1 - \log(2 - x^2)\right] \\[2ex]
\text{Boundary Conditions:} \begin{cases} x = 0 : \dfrac{\partial u}{\partial x} = 0 \\[2ex] x = 1 : u = 2 + \log(1 + t) \end{cases} \\[2ex]
\text{Exact Solution:} \quad u = 2 + \log(1 + t) - 2\log(2 - x^2)
\end{array}\right\} \qquad (75)$$

Using higher-order central differences when replacing $\frac{\partial^2 u}{\partial x^2}$ by finite differences, the partial differential equation of our problem is converted into the following system of ordinary differential equations:

$$\left.\begin{array}{l}
\dfrac{du_i(\tau)}{d\tau} = \dfrac{1}{4} \cdot \dfrac{e^2}{2 + x_i^2} \cdot e^{-u_i(\tau)} \Big\{ \delta^2 u_i(\tau) - \dfrac{1}{12}\delta^4 u_i(\tau) \\[2ex]
\qquad\qquad\qquad\qquad\qquad + \dfrac{1}{90}\delta^6 u_i(\tau) - + \ldots \Big\}
\end{array}\right\} \qquad (76)$$

The introduction of the fourth-, sixth-, . . . order differences in (76) makes necessary some extrapolation in the vicinity of the boundary line $x = 1$. When including the fourth-order differences only, we have assumed that the sixth-order differences are constant in the vicinity of $x = 1$. Correspondingly, the eighth-order differences are assumed to be constant if sixth-order differences are still carried in (76). For $x = 0$ no extrapolation is needed since the problem is symmetric with respect to $x = 0$.

For our computation we divided the x-interval $< 0, 1 >$ into 16 equal parts $(h = \frac{1}{16})$. The numerical integration of (76) with respect to $\tau = \frac{t}{h^2}$ was performed with a tolerance of 10^{-8} on an eight-decimal digit computer. The stepsize control procedure was applied for $x = 0$ only.

Table XVII shows the results for $t = 100$, obtained with some of our new formulas. Under the heading "Method" of Table XVII we have also indicated the order of the highest central difference δ^2, δ^4, or δ^6 carried in (76).

TABLE XVII. COMPARISON OF VARIOUS RUNGE-KUTTA METHODS FOR PROBLEM (75)

Results for t = 100 (Tolerance: 10^{-8}; $h = \frac{1}{16}$)

Method	Order of Method	Number of Steps	Running Time (min) on IBM-7094	Accumulated Error (maximum) in u
EULER-CAUCHY (Table XV) — δ^2	1	30 721	1.75	$0.1408 \cdot 10^{-2}$
RK1(2) (Table XIV) — δ^2	1	1 924	0.22	$0.1452 \cdot 10^{-2}$
RK2(3) (Table XI) — δ^2	2	822	0.23	$0.1425 \cdot 10^{-2}$
RK3(4) (Table VIII) — δ^2	3	1 036	0.33	$0.1424 \cdot 10^{-2}$
EULER-CAUCHY (Table XV) — δ^4	1	30 715	2.07	$-0.3767 \cdot 10^{-4}$
RK1(2) (Table XIV) — δ^4	1	1 998	0.28	$-0.1991 \cdot 10^{-4}$
RK2(3) (Table XI) — δ^4	2	1 070	0.36	$-0.1961 \cdot 10^{-4}$
RK3(4) (Table VIII) — δ^4	3	1 305	0.50	$-0.2086 \cdot 10^{-4}$
EULER-CAUCHY (Table XV) — δ^6	1	30 712	2.33	$-0.2068 \cdot 10^{-4}$
RK1(2) (Table XIV) — δ^6	1	2 072	0.39	$-0.1848 \cdot 10^{-5}$
RK2(3) (Table XI) — δ^6	2	1 227	0.45	$-0.3636 \cdot 10^{-5}$
RK3(4) (Table VIII) — δ^6	3	1 520	0.61	$-0.4947 \cdot 10^{-5}$

From Table XVII one recognizes immediately the gain of accuracy obtained by taking into account the fourth- and sixth-order central differences in (76). The results clearly suggest that at least the fourth-order central differences should be included in the computation.

The table also shows that our new RUNGE-KUTTA methods give about the same or more accurate results in a fraction of the time required by EULER-CAUCHY's method, which is identical with the explicit difference formula (69).

However, our third-order formula is already slower on the computer than our first- and second-order formulas. The trend continues: our fourth-order formula is again slower than our third-order formula, etc.

This confirms the experience that other authors have had with fourth-order RUNGE-KUTTA formulas, which are too slow for heat transfer problems and cannot compete with our new lower-order RUNGE-KUTTA formulas.

50. We present another example:

Second problem:

$$\left.\begin{aligned}
&\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + 2t \cdot \frac{\partial u}{\partial x} + u\,[(\log u)^2 + \log u - 1] \\
&\text{Initial Condition:} \quad t = 0 : u = e^{\cos x} \\
&\text{Boundary Conditions:} \quad \begin{cases} x = 0 : u = e^{\cos(t^2)} \\ x = 1 : u = e^{\cos(1+t^2)} \end{cases} \\
&\text{Exact Solution:} \quad u = e^{\cos(x+t^2)}
\end{aligned}\right\} \quad (77)$$

In this example we have to replace $\frac{\partial u}{\partial x}$ by finite differences also. Taking into account higher-order central differences, we replace the partial differential equation of our problem with the following system of ordinary differential equations:

$$\left.\begin{aligned}
\frac{du_i(\tau)}{d\tau} = {} & \left[\delta^2 u_i(\tau) - \frac{1}{12}\delta^4 u_i(\tau) + \frac{1}{90}\delta^6 u_i(\tau)\right] \\
& + h^3 \circ \tau \left[\left(u_{i+1}(\tau) - u_{i-1}(\tau)\right) - \frac{1}{6}\left(\delta^2 u_{i+1}(\tau) - \delta^2 u_{i-1}(\tau)\right)\right. \\
& \qquad \left. + \frac{1}{30}\left(\delta^4 u_{i+1}(\tau) - \delta^4 u_{i-1}(\tau)\right)\right] \\
& + h^2 \cdot u_i(\tau) \left[\left(\log u_i(\tau)\right)^2 + \log u_i(\tau) - 1\right]
\end{aligned}\right\} \quad (78)$$

The numerical integration of (78) is performed in the same way as in our first problem. However, our new problem requires some extrapolating for $x = 0$ also; and the stepsize control procedure is now performed for $x = \frac{1}{2}$.

Table XVIII shows our results for t = 5. These results are quite similar to those for our first problem. The computer time for our new RUNGE-KUTTA formulas is, however, here a considerably smaller fraction of the computer time of the explicit difference formula (EULER-CAUCHY's formula).

TABLE XVIII. COMPARISON OF VARIOUS RUNGE-KUTTA METHODS FOR PROBLEM (77)

Method	Order of Method	Number of Steps	Running Time (min) on IBM-7094	Accumulated Error (maximum) in u
		Results for $t = 5$ $\left(\text{Tolerance: } 10^{-8};\ h = \frac{1}{16}\right)$		
EULER-CAUCHY (Table XV) — δ^2	1	235 354	19.46	$0.6313 \cdot 10^{-3}$
RK1(2) (Table XIV) — δ^2	1	14 737	2.47	$0.6711 \cdot 10^{-3}$
RK2(3) (Table XI) — δ^2	2	2 142	0.87	$0.7065 \cdot 10^{-3}$
RK3(4) (Table VIII) — δ^2	3	2 519	1.03	$0.6745 \cdot 10^{-3}$
EULER-CAUCHY (Table XV — δ^4	1	235 388	22.87	$-0.4032 \cdot 10^{-4}$
RK1(2) (Table XIV) — δ^4	1	14 906	2.93	$-0.3516 \cdot 10^{-5}$
RK2(3) (Table XI) — δ^4	2	2 695	1.08	$0.3994 \cdot 10^{-5}$
RK3(4) (Table VIII) — δ^4	3	3 334	1.91	$0.3129 \cdot 10^{-5}$
EULER-CAUCHY (Table XV) — δ^6	1	235 372	25.32	$-0.5391 \cdot 10^{-5}$
RK1(2) (Table XIV) — δ^6	1	14 971	3.25	$-0.4351 \cdot 10^{-5}$
RK2(3) (Table XI) — δ^6	2	2 812	1.50	$-0.3427 \cdot 10^{-5}$
RK3(4) (Table VIII) — δ^6	3	3 677	2.38	$-0.1132 \cdot 10^{-5}$

51. In both examples, our new low-order RUNGE-KUTTA formulas proved to be considerably faster and of equal or better accuracy than the conventional explicit difference formula (69). This is not too suprising if one realizes that (69) is a formula of first-order accuracy only, and that its truncation error factor is 256 times as large as the error factor of our first-order formula RK1(2) of Table XIV.

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