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Limiting Formulas of Nine-stage Explicit Runge–Kutta Methods of Order Eight

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The attainable order of a nine-stage explicit Runge–Kutta formula is at most seven. However, by taking the limit as the distance between the first two and the last two abscissas approaches zero, the formula can achieve eighth order. In this paper, a family of nine-stage eighth-order limiting formulas with four free parameters is derived. Every other parameter is represented as a fractional expression using one or more of these free parameters. Two examples of the method are presented. One of them has a considerably large stability region, but its parameters require a large number of digits. The other has parameters requiring a comparatively small number of digits, but its stability region is not so large.

1. Introduction

The attainable order p of s-stage explicit Runge–Kutta methods is $s-1$ for $s=5$, $s=6$, and $s=7$, and is $s-2$ for $s=8$ and $s=9$. However, they can achieve order $p+1$ in the limiting case where the distance between some pairs of abscissas approaches zero. Such formulas are called limiting formulas. They require evaluation of the derivatives in addition to evaluation of the function. Five-stage fifth-order[14], six-stage sixth-order[7] and eight-stage seventh-order[8] limiting formulas have been derived.

In this paper, a family of nine-stage eighth-order limiting formulas is presented. It is derived in a similar way to the six-stage case. The nine-stage eighth-order limiting formula has four free parameters. Every other parameter is represented as a fractional expression using one or more of them. The polynomial that determines the stability region is a function of one of the free parameters. Thus, we can obtain various formulas by choosing the values of these free parameters to take account of the properties of the formula. The values of the product of the Jacobian matrix and the vector involved in this formula can be easily calculated by using automatic differentiation[5),10].

Here, two recommendable sets of free parameters and the methods corresponding to these sets are given. One of them has a fairly large stability region, but its parameters require a large number of digits. The other method's stability region is not so large, but the numerators and denominators of the coefficients of this method are numbers with a comparatively small number of digits. The latter method is one of the most efficient methods for non-stiff systems, because high-order explicit Runge–Kutta methods are not used for stiff systems.

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2. Limiting Formulas

We will consider the system of the initial value problem

$$\frac{dy}{dt} = f(t,y), \quad y(t_0) = y_0,$$

where f and y are vectors and f is assumed to be differentiable sufficiently often for the definition to be meaningful. The parameters of an s-stage explicit Runge–Kutta method are represented in the following Butcher array[3]:

$$\begin{array}{c|cccc} c_2 & a_{21} & & & \\ c_3 & a_{31} & a_{32} & & \\ \vdots & \vdots & & \ddots & \\ c_s & a_{s1} & a_{s2} & \cdots & a_{s,s-1} \\ \hline & b_1 & b_2 & \cdots & & b_s. \end{array}$$

The method is written in the form

$$f_1 = f(t_n, y_n), \quad y_i = y_n + h\sum_{j=1}^{i-1} a_{ij} f_j,$$

$$f_i = f(t_n + c_i h, y_i) \quad (i = 2, 3, \cdots, s)$$

$$y_{n+1} = y_n + h\sum_{1=1}^{s} b_i f_i.$$

The properties of nine-stage seventh-order formulas are precisely reported and some effective formulas are proposed by Tanaka, et al.[12),13]. A minute observation of his formulas shows that the truncation error of the formula

Table 1 Limiting formulas.

Stage	Limiting formula	Abscissa
5	5th-order	$c_2 \to 0$
	5th-order	$c_4 \to c_5 = 1$
6	6th-order	$c_2 \to 0$ and $c_5 \to c_6 = 1$
7	7th-order	$c_2, c_3 \to 0,$ and $c_6 \to c_7 = 1$
8	7th-order	$c_2 \to 0$

become small as the abscissa c_2 approaches zero and c_8 approaches c_9 $(= 1)$ simultaneously. Thus, it is expected that a nine-stage formula can achieve eighth-order in the limiting case where c_2 tends to 0 and c_8 tends to c_9 $(= 1)$. Limiting formulas that use the values of derivatives were derived for five stages by Toda[14], for six stages and for eight stages by Ono[7),8)], and for seven stages by Ono and Toda[9]. They are listed in **Table 1**.

A nine-stage limiting formula will have a form similar to the six-stage limiting formula:

$$f_1 = f(t_n, y_n), \quad F_2 = D(f(t_n, y_n)) \cdot v(f_1),$$
$$y_3 = y_n + h(a_{31} f_1 + h\alpha_3 F_2), \; f_3 = f(t_n + c_3 h, y_3),$$
$$y_i = y_n + h\left(\sum_{j=1,\neq 2}^{i-1} a_{ij} f_j + h\alpha_i F_2\right),$$
$$f_i = f(t_n + c_i h, y_i) \qquad (i = 4, 5, \cdots, 8),$$
$$\tilde{f}_9 = \sum_{j=1,\neq 2}^{8} A_{9j} f_j + h\alpha_9 F_2,$$
$$F_9 = D(f(t_n + h, y_8)) \cdot v(\tilde{f}_9),$$
$$y_{n+1} = y_n + h\left(\sum_{i=1,\neq 2}^{8} b_i f_i + h\beta_2 F_2 + h\beta_9 F_9\right), \tag{1}$$

where $D(f(t_p, y_p))$ denotes the Jacobian matrix of f at the point (t_p, y_p), $v(f_1)$ denotes the vector $(1, f_1^1, f_1^2, \cdots, f_1^n)^T$, and $v(\tilde{f}_9)$ denotes the vector $(1, \tilde{f}_9^1, \tilde{f}_9^2, \cdots, \tilde{f}_9^n)^T$ (the superscripts denote the component numbers). The parameters of this limiting formula can be written in the following array analogous to the Butcher array:

$$\begin{array}{c|cccccc|c}
c_3 & a_{31} & & & & & & \alpha_3 \\
c_4 & a_{41} & a_{43} & & & & & \alpha_4 \\
c_5 & a_{51} & a_{53} & a_{54} & & & & \alpha_5 \\
\vdots & \vdots & & & \ddots & & & \vdots \\
c_8 & a_{81} & a_{83} & a_{84} & \cdots & a_{87} & & \alpha_8 \\
 & A_{91} & A_{93} & A_{94} & \cdots & A_{97} & A_{98} & \alpha_9 \\
\hline
 & b_1 & b_3 & b_4 & \cdots & & b_8 & \\
 & \beta_2 & \beta_9 & & & & &
\end{array}$$

The relations between the parameters of limiting formulas and those of usual nine-stage formulas are as follows:

Limiting formula	Usual nine-stage formula
a_{i1}	$\lim_{c_2 \to 0}(a_{i1} + a_{i2}) \quad (i = 3, \cdots, 8)$
α_i	$\lim_{c_2 \to 0} a_{i2} c_2 \quad (i = 3, \cdots, 7)$
A_{91}	$\lim_{c_8 \to 1}(\lim_{c_2 \to 0}(a_{91} + a_{92} - (a_{81} + a_{82}))/(1 - c_8))$
A_{9j}	$\lim_{c_8 \to 1}(a_{9j} - a_{8j})/(1 - c_8) \quad (j = 3, \cdots, 7)$
A_{98}	$\lim_{c_8 \to 1} a_{98}/(1 - c_8)$
α_9	$\lim_{c_8 \to 1}(\lim_{c_2 \to 0}(a_{92}c_2 - a_{82}c_2)/(1 - c_8))$
b_1	$\lim_{c_2 \to 0}(b_1 + b_2)$
b_8	$\lim_{c_8 \to 1}(b_8 + b_9)$
β_2	$\lim_{c_2 \to 0} b_2 c_2$
β_9	$\lim_{c_8 \to 1}(-b_8(1 - c_8))$

2.1 Order Conditions

We shall restrict ourselves to the case in which $b_3 = 0$ and the following simplifying assumptions hold:

$$c_8 = 1, \quad \alpha_3 = \frac{c_3^2}{2}, \quad \sum_{j=3}^{i-1} a_{ij} c_j + \alpha_i = \frac{c_i^2}{2},$$
$$\sum_{j=3}^{i-1} a_{ij} c_j^2 = \frac{c_i^3}{3} \quad (i = 4, 5, \cdots, 8). \tag{2}$$

Comparing the Taylor series expansion of Eq. (1) with that of the true value $y(t_n + h)$ and matching the coefficients of each elementary differential, after tedious computation, we obtain the following equations of the order conditions:

$$a_{31} = c_3, \quad a_{i1} + \sum_{j=3}^{i-1} a_{ij} = c_i \quad (i = 4, 5, \cdots, 8),$$
$$A_{91} + \sum_{j=3}^{8} A_{9,j} = 1, \quad \alpha_9 + \sum_{j=3}^{8} A_{9,j} c_j = 1, \tag{3}$$
$$\sum_{i=j+1}^{8} b_i a_{ij} + \beta_9 A_{9j} = b_j(1 - c_j) \; (j = 4, 5, 6, 7),$$
$$\beta_9 A_{98} = -\beta_9, \tag{4}$$
$$\sum_{i=4}^{8} b_i a_{i3} + \beta_9 A_{93} = 0, \tag{5}$$
$$\sum_{i=5}^{8} b_i \sum_{j=4}^{i-1} a_{ij} a_{j3} + \beta_9 \sum_{j=4}^{8} A_{9j} a_{j3} = 0, \tag{6}$$
$$\sum_{i=6}^{8} b_i \sum_{j=5}^{i-1} a_{ij} \sum_{k=4}^{j-1} a_{jk} a_{k3} + \beta_9 \sum_{j=5}^{8} A_{9j} \sum_{k=4}^{j-1} a_{jk} a_{k3} = 0, \tag{7}$$

$$\sum_{i=7}^{8} b_i \sum_{j=6}^{i-1} a_{ij} \sum_{k=5}^{j-1} a_{jk} \sum_{l=4}^{k-1} a_{kl} a_{l3} + \beta_9 \sum_{j=6}^{8} A_{9j} \sum_{k=5}^{j-1} a_{jk} \sum_{l=4}^{k-1} a_{kl} a_{l3} = 0, \quad (8)$$

$$\sum_{i=6}^{8} b_i \sum_{j=5}^{i-1} a_{ij} \sum_{k=4}^{j-1} a_{jk} c_k a_{k3} + \beta_9 \sum_{j=5}^{8} A_{9j} \sum_{k=4}^{j-1} a_{jk} c_k a_{k3} = 0, \quad (9)$$

$$b_1 + \sum_{i=4}^{8} b_i = 1, \quad \sum_{i=4}^{8} b_i c_i + \beta_2 + \beta_9 = \frac{1}{2}, \quad (10)$$

$$\sum_{i=4}^{8} b_i c_i^2 + 2\beta_9 = \frac{1}{3}, \quad (11)$$

$$\sum_{i=5}^{8} b_i \sum_{j=4}^{i-1} a_{ij} c_j^2 + \beta_9 \sum_{j=4}^{8} A_{9j} c_j^2 = \frac{1}{12}, \quad (12)$$

$$\sum_{i=5}^{8} b_i \sum_{j=4}^{i-1} a_{ij} c_j^3 + \beta_9 \sum_{j=4}^{8} A_{9j} c_j^3 = \frac{1}{20}, \quad (13)$$

$$\sum_{i=5}^{8} b_i \sum_{j=4}^{i-1} a_{ij} c_j^4 + \beta_9 \sum_{j=4}^{8} A_{9j} c_j^4 = \frac{1}{30}, \quad (14)$$

$$\sum_{i=6}^{8} b_i \sum_{j=5}^{i-1} a_{ij} \sum_{k=4}^{j-1} a_{jk} c_k^3 + \beta_9 \sum_{j=5}^{8} A_{9j} \sum_{k=4}^{j-1} a_{jk} c_k^3 = \frac{1}{120}, \quad (15)$$

$$\sum_{i=5}^{8} b_i \sum_{j=4}^{i-1} a_{ij} c_j^5 + \beta_9 \sum_{j=4}^{8} A_{9j} c_j^5 = \frac{1}{42}, \quad (16)$$

$$\sum_{i=6}^{8} b_i \sum_{j=5}^{i-1} a_{ij} \sum_{k=4}^{j-1} a_{jk} c_k^4 + \beta_9 \sum_{j=5}^{8} A_{9j} \sum_{k=4}^{j-1} a_{jk} c_k^4 = \frac{1}{210}, \quad (17)$$

$$\sum_{i=7}^{8} b_i \sum_{j=6}^{i-1} a_{ij} \sum_{k=5}^{j-1} a_{jk} \sum_{l=4}^{k-1} a_{kl} c_l^3 + \beta_9 \sum_{j=6}^{8} A_{9j} \sum_{k=5}^{j-1} a_{jk} \sum_{l=4}^{k-1} a_{kl} c_l^3 = \frac{1}{840}, \quad (18)$$

$$\sum_{i=6}^{8} b_i \sum_{j=5}^{i-1} a_{ij} c_j \sum_{k=4}^{j-1} a_{jk} c_k^3 + \beta_9 \sum_{j=5}^{8} A_{9j} c_j \sum_{k=4}^{j-1} a_{jk} c_k^3 = \frac{1}{168}, \quad (19)$$

$$\sum_{i=5}^{8} b_i \sum_{j=4}^{i-1} a_{ij} c_j^6 + \beta_9 \sum_{j=4}^{8} A_{9j} c_j^6 = \frac{1}{56}, \quad (20)$$

$$\sum_{i=6}^{8} b_i \sum_{j=5}^{i-1} a_{ij} \sum_{k=4}^{j-1} a_{jk} c_k^5 + \beta_9 \sum_{j=5}^{8} A_{9j} \sum_{k=4}^{j-1} a_{jk} c_k^5 = \frac{1}{336}, \quad (21)$$

$$\sum_{i=7}^{8} b_i \sum_{j=6}^{i-1} a_{ij} \sum_{k=5}^{j-1} a_{jk} \sum_{l=4}^{k-1} a_{kl} c_l^4 + \beta_9 \sum_{j=6}^{8} A_{9j} \sum_{k=5}^{j-1} a_{jk} \sum_{l=4}^{k-1} a_{kl} c_l^4 = \frac{1}{1680}, \quad (22)$$

$$b_8 a_{87} a_{76} a_{65} a_{54} c_4^3 + \beta_9 \sum_{j=7}^{8} A_{9j} \sum_{k=6}^{j-1} a_{jk} \sum_{l=5}^{k-1} a_{kl} \sum_{m=4}^{l-1} a_{lm} c_m^3 = \frac{1}{6720}, \quad (23)$$

$$\sum_{i=6}^{8} b_i \sum_{j=5}^{i-1} a_{ij} c_j \sum_{k=4}^{j-1} a_{jk} c_k^4 + \beta_9 \sum_{j=5}^{8} A_{9j} c_j \sum_{k=4}^{j-1} a_{jk} c_k^4 = \frac{1}{280}, \quad (24)$$

$$\sum_{i=6}^{8} b_i \sum_{j=5}^{i-1} a_{ij} c_j^2 \sum_{k=4}^{j-1} a_{jk} c_k^3 + \beta_9 \sum_{j=5}^{8} A_{9j} c_j^2 \sum_{k=4}^{j-1} a_{jk} c_k^3 = \frac{1}{224}, \quad (25)$$

$$\sum_{i=7}^{8} b_i \sum_{j=6}^{i-1} a_{ij} c_j \sum_{k=5}^{j-1} a_{jk} \sum_{l=4}^{k-1} a_{kl} c_l^3 + \beta_9 \sum_{j=6}^{8} A_{9j} c_j \sum_{k=5}^{j-1} a_{jk} \sum_{l=4}^{k-1} a_{kl} c_l^3 = \frac{1}{1120}, \quad (26)$$

$$\sum_{i=7}^{8} b_i \sum_{j=6}^{i-1} a_{ij} \sum_{k=5}^{j-1} a_{jk} c_k \sum_{l=4}^{k-1} a_{kl} c_l^3 + \beta_9 \sum_{j=6}^{8} A_{9j} \sum_{k=5}^{j-1} a_{jk} c_k \sum_{l=4}^{k-1} a_{kl} c_l^3 = \frac{1}{1344}. \quad (27)$$

2.2 Solutions

In this section, we assume that abscissas c_i ($i = 4, 5, 6, 7$) are distinct and are not equal to 0 and 1. We define, for later convenience, the following auxiliary parameters:

$$\sum_{i=j+1}^{8} b_i a_{ij} + \beta_9 A_{9j} = b_j(1 - c_j) \stackrel{\text{def}}{=} \rho_j \ (j = 4, 5, 6, 7),$$

$$\beta_9 A_{98} = \rho_8, \quad \sum_{j=k+1}^{8} \rho_j a_{jk} \overset{\text{def}}{=} \sigma_k \ (k = 4,5,6,7),$$

$$\sum_{k=l+1}^{7} \sigma_k a_{kl} \overset{\text{def}}{=} \tau_l \ (l{=}4,5,6), \sum_{k=l+1}^{6} \tau_k a_{kl} \overset{\text{def}}{=} \phi_l \ (l{=}4,5). \quad (28)$$

The outline of the derivation is shown in the appendix. Here we show only the results. Rewriting the equations of the order conditions by using Eq. (28), we obtain

$$\rho_i = \frac{28c_jc_kc_l - 14(c_kc_l + c_jc_l + c_jc_k) + 8(c_j + c_k + c_l) - 5}{840c_i^2(c_i - c_j)(c_i - c_k)(c_i - c_l)(c_i - 1)}$$

$$\rho_8 = (70c_ic_jc_kc_l - 42\textstyle\sum_{i,j,k} c_ic_jc_k + 28\sum_{i,j} c_ic_j - 20\sum_i c_i + 15)$$
$$/(840(1 - c_4)(1 - c_5)(1 - c_6)(1 - c_7)),$$

$$\sigma_i = \frac{\rho_i(1 - c_i)}{2} \qquad (i, j, k, l = 4, 5, 6, 7),$$

$$\tau_i = \frac{14c_jc_k - 6(c_j + c_k) + 3}{5040c_i^2(c_i - c_j)(c_i - c_k)} \ (i, j, k = 4, 5, 6),$$

$$\phi_i = \frac{-8c_j + 3}{20160c_i^2(c_i - c_j)} \quad (i, j = 4, 5), \qquad (29)$$

and the relation between c_4 and c_5, which must be satisfied:

$$(56c_4^2 - 42c_4 + 9)c_5 - 3c_4 = 0. \qquad (30)$$

If we assume that the values of c_i are in the interval $(0, 1)$, then from (30) we get

$$0 < c_4 < \frac{3}{8} \quad \text{or} \quad \frac{3}{7} < c_4 < 1. \qquad (31)$$

All parameters of the method can be obtained successively in terms of c_i using ρ_i, σ_i, τ_i, and ϕ_i, provided that all denominators do not vanish. The parameters b_i and β_i are

$$b_i = \frac{\rho_i}{(1 - c_i)} \ (i = 4, 5, 6, 7), \ \beta_9 = -\rho_8,$$

$$b_8 = \frac{1}{3} - (\textstyle\sum_{i=4}^{7} b_ic_i^2 + 2\beta_9), \ b_1 = 1 - \sum_{i=4}^{8} b_i,$$

$$\beta_2 = \frac{1}{2} - (\textstyle\sum_{i=4}^{8} b_ic_i + \beta_9), \qquad (32)$$

and a_{ij} and $A_{9j} (j = 8, 7, 6, 5, 4)$ are

$$A_{98} = -1, \ a_{87} = \frac{\sigma_7}{\rho_8}, \ A_{97} = \frac{\rho_7 - b_8a_{87}}{\beta_9}, \ a_{76} = \frac{\tau_6}{\sigma_7},$$

$$a_{86} = \frac{\sigma_6 - \rho_7a_{76}}{\rho_8}, \ A_{96} = \frac{\rho_6 - \sum_{i=7}^{8} b_ia_{i6}}{\beta_9},$$

$$a_{65} = \frac{\phi_5}{\tau_6}, \quad a_{75} = \frac{\tau_5 - \sigma_6a_{65}}{\sigma_7},$$

$$a_{85} = \frac{\sigma_5 - \sum_{i=6}^{7} \rho_ia_{i5}}{\rho_8}, \ A_{95} = \frac{\rho_5 - \sum_{i=6}^{8} b_ia_{i5}}{\beta_9},$$

$$a_{54} = \frac{c_5^3(c_5 - c_4)}{c_4^3}, \quad a_{64} = \frac{\phi_4 - \tau_5a_{54}}{\tau_6},$$

$$a_{74} = \frac{\tau_4 - \sum_{i=5}^{6} \sigma_ia_{i4}}{\sigma_7}, \ a_{84} = \frac{\sigma_4 - \sum_{i=5}^{7} \rho_ia_{i4}}{\rho_8},$$

$$A_{94} = \frac{\rho_4 - \sum_{i=5}^{8} b_ia_{i4}}{\beta_9}. \qquad (33)$$

Finally, a_{i3}, $A_{9j} (j = 3, 1)$, α_i, and a_{i1} are

$$a_{43} = \frac{c_4^3}{3c_3^2}, \ a_{i3} = \frac{c_i^3 - 3\sum_{j=4}^{i-1} a_{ij}c_j^2}{3c_3^2} \ (i = 5, 6, 7, 8),$$

$$A_{93} = -\frac{\sum_{i=4}^{8} b_ia_{i3}}{\beta_9}, \ A_{91} = 1 - \sum_{j=3}^{8} A_{9j}, \ \alpha_3 = \frac{c_3^2}{2},$$

$$\alpha_i = \frac{c_i^2}{2} - \sum_{j=3}^{i-1} a_{ij}c_j \ (i = 4, 5, \cdots, 8), \alpha_9 = 1 - \sum_{j=3}^{8} A_{9j}c_j,$$

$$a_{31} = c_3, \ a_{i1} = c_i - \sum_{j=3}^{i-1} a_{ij} \ (i = 4, 5, \cdots, 8). \quad (34)$$

Now, we have obtained a set of parameters of the nine-stage eighth-order limiting formula with four free parameters, c_3, c_4, c_6, and c_7.

3. Determination of the Free Parameters

In this section we will consider how to determine the four free parameters. The stability region depends on only one free parameter, c_4. It is desirable to determine c_4 so as to maximize the stability region. At the same time, it is preferable that every parameter be a number that requires a small number of digits and has a small magnitude. Here, we will present two sets of free parameters. Substituting the values of these sets into the solutions obtained in the previous section, we obtain two formulas. One of them has a comparatively large stability region, and the other has relatively simple numbers as parameters.

3.1 Stability

The polynomial r that determines the stability region of the nine-stage eighth-order limiting formula (1) is given by

$$r(z) = 1 + z + \frac{z^2}{2!} + \frac{z^3}{3!} + \cdots + \frac{z^7}{7!} + \frac{z^8}{8!} + \gamma z^9,$$

where z is a complex number and

$$\gamma = \phi_5a_{54}a_{43}\alpha_3 = \frac{c_4(3 - 8c_4)}{40320(56c_4^2 - 42c_4 + 9)}.$$

Let the simply connected interval $(-d, 0)$ be the intersection of the stability region and the negative part of the real axis. The stability boundaries for several values of γ are shown in **Fig. 1**. The graph indicates that

$$\gamma \in \left(\frac{1}{620000}, \frac{1}{580000}\right) \qquad (35)$$

gives the maximum stability region. The graph of $\gamma(c_4)$ for the interval (31) is given in **Fig. 2**. The intervals for c_4, for which γ is in the interval

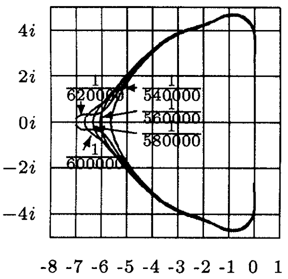

Fig. 1 Stability boundaries for several values of γ.

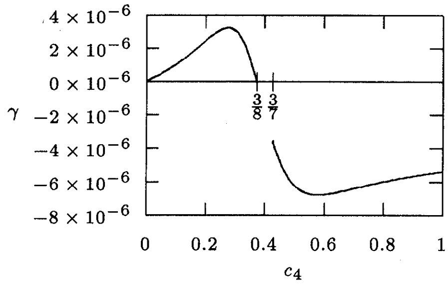

Fig. 2 Graph of $\gamma(c_4)$ for $0 < c_4 < 3/8$ and $3/7 < c_4 < 1$.

(35), are approximately

$$.1446 < c_4 < .1523 \text{ and } .3455 < c_4 < .3477. \quad (36)$$

3.2 Two Sets of Free Parameters

To find a method that has a comparatively large stability region, we will proceed as follows: (i) Let the rational number be a value of c_4 that lies within the intervals given in Eq. (36) and whoes numerator and denominator are numbers with at most two digits. (ii) For all such values of c_4, we look for a value of c_5 whose numerator and denominator are also numbers with at most two digits (the value of c_5 is determined by relation (30)). (iii) For every such pair of (c_4, c_5) and the values of c_6 and c_7 $(0 < c_6, c_7 < 1)$, we look for the minimum s, the sum of the magnitude of the parameters in Eqs. (32) and (33), because these parameters are independent of the value of c_3. (iv) As the values of c_6 and c_7, we choose the simplest pair of numbers near the pair of c_6 and c_7 that gives the minimum s. (v) Finally, we look for the value of c_3 in a similar way; that is, we look for the minimum sum of the magnitude of the parameters (34). We determine the simplest rational number as the value of c_3 that gives nearly the minimum sum. Thus we obtain a set of free parameters:

$$c_3 = \frac{1}{3}, \ c_4 = \frac{9}{26}, \ c_6 = \frac{3}{4}, \ c_7 = \frac{1}{4}. \quad (37)$$

For this set, the values of c_5, γ, and d are

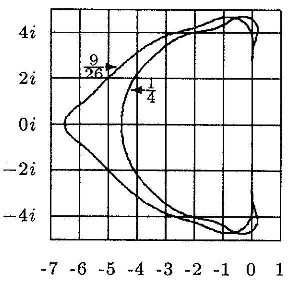

Fig. 3 Stability boundaries for $c_4 = 9/26$ and $1/4$.

$$c_5 = \frac{39}{44}, \ \gamma = \frac{1}{591360} \approx 1.691 \times 10^{-6}, \ d \approx 6.5.$$

We will give another value of c_4 for which all the parameters have a relatively small number of digits. First, we look for the pair of c_4 and c_5 such that all numerators and denominators are numbers with one digit. We determine 1/4 as the value of c_4, because it gives the largest stability region among such pairs. Then, we proceed as for $c_4 = 9/26$, and get

$$c_3 = \frac{1}{4}, \ c_4 = \frac{1}{4}, \ c_6 = \frac{7}{8}, \ c_7 = \frac{3}{4}. \quad (38)$$

For this set, the values of c_5, γ, and d are

$$c_5 = \frac{3}{8}, \ \gamma = \frac{1}{322560} \approx 3.100 \times 10^{-6}, \ d \approx 4.5.$$

This value of c_4 is outside of the intervals in Eq. (36). Thus, the stability region is not so large, but the parameters of the formula require a far smaller number of digits than that for $c_4 = 9/26$. The stability boundaries for these two values of c_4, 9/26 and 1/4, are shown in **Fig. 3**.

3.3 Nine-stage Eighth-order Limiting Formulas

Substituting the set of c_i (38) into Eqs. (29), (32), (33), and (34), we obtain Formula 1. The stability region of this formula is not so large, but its parameters are numbers that require a comparatively small number of digits. The parameters of this formula are shown in **Table 2**.

For the set of c_i (37), we obtain Formula 2. This formula has a comparatively large stability region, but its parameters are more complicated than those of Formula 1. The parameters of Formula 2 are shown in **Table 3**.

4. Numerical Example and Conclusions

We will show that our derivations are correct. First, our formula is definitely eight-order. Though this can be verified by substituting the values from Table 2 and Table 3 into the error coefficients up to $O(h^8)$ terms, here we will

Table 2 Formula 1.

c_i	a_{ij} $(i=3,4,\cdots,8; j=1,3,\cdots,8)$							α_i
$\frac{1}{4}$	$\frac{1}{4}$							$\frac{1}{32}$
$\frac{1}{4}$	$\frac{1}{6}$	$\frac{1}{12}$						$\frac{1}{96}$
$\frac{3}{8}$	$\frac{3}{32}$	$-\frac{9}{64}$	$\frac{27}{64}$					0
$\frac{7}{8}$	$\frac{12607}{2592}$	$\frac{2303}{576}$	$-\frac{2695}{192}$	$\frac{490}{81}$				$\frac{539}{864}$
$\frac{3}{4}$	$\frac{2297}{2058}$	$\frac{3}{4}$	$-\frac{207}{70}$	$\frac{38}{21}$	$\frac{54}{1715}$			$\frac{199}{1568}$
1	$\frac{32183}{8967}$	$\frac{832}{183}$	$-\frac{600}{61}$	$\frac{320}{183}$	$-\frac{1728}{2989}$	$\frac{280}{183}$		$\frac{1345}{2562}$
A_{9j}	$\frac{16106722}{1640961}$	$\frac{150016}{3721}$	$-\frac{470864}{18605}$	$-\frac{1243520}{33489}$	$-\frac{7922304}{911645}$	$\frac{770224}{33489}$	-1	$\frac{65822}{26047}$
b_j	$\frac{12289}{92610}$	0	$\frac{704}{4725}$	$\frac{2048}{7875}$	$-\frac{2048}{8575}$	$\frac{64}{135}$	$\frac{10537}{47250}$	
β_2, β_9	$\frac{47}{8820}$	$-\frac{61}{6300}$						

Table 3 Formula 2.

c_i	a_{ij} $(j=1,3,\cdots,8)$							α_i
$\frac{1}{3}$	$\frac{1}{3}$							$\frac{1}{18}$
$\frac{9}{26}$	$\frac{3897}{17576}$	$\frac{2187}{17576}$						$\frac{81}{4394}$
$\frac{39}{44}$	$-\frac{8292271}{16866432}$	$-\frac{14414517}{1874048}$	$\frac{38243179}{4216608}$					$-\frac{342563}{1874048}$
$\frac{3}{4}$	$-\frac{349085}{3699072}$	$-\frac{3159}{2432}$	$\frac{1184183}{563616}$	$\frac{27951}{661466}$				$-\frac{1597}{31616}$
$\frac{1}{4}$	$\frac{63001339}{299624832}$	$-\frac{351}{2432}$	$\frac{7986095}{45652896}$	$-\frac{1164625}{53578746}$	$\frac{5}{162}$			$\frac{38219}{2560896}$
1	$-\frac{3578509}{8993673}$	$-\frac{702}{73}$	$\frac{328398772}{38369457}$	$-\frac{363416240}{720493137}$	$\frac{48640}{41391}$	$\frac{912}{511}$		$-\frac{21163}{153738}$
A_{9j}	$-\frac{16288620394}{3720382731}$	$-\frac{7275528}{90593}$	$\frac{3275107674488}{79360826895}$	$-\frac{2097338476640}{298043994339}$	$\frac{281776384}{17122077}$	$\frac{114146528}{3170755}$	-1	$-\frac{19731878}{31798143}$
b_j	$\frac{1202603}{8624070}$	0	$\frac{501988136}{1563686775}$	$-\frac{2494357888}{8636047875}$	$\frac{9728}{19845}$	$\frac{2432}{33075}$	$\frac{212561}{803250}$	
β_2, β_9	$\frac{857}{147420}$	$-\frac{73}{6300}$						

give a simpler demonstration using a numerical example. We give the errors in the numerical solution of a system of equations[2]:

Example 1: Integrate

$$\frac{dy_1}{dt} = y_2 y_3, \qquad y_1(0) = 0,$$
$$\frac{dy_2}{dt} = -y_1 y_3, \qquad y_2(0) = 1,$$
$$\frac{dy_3}{dt} = -k^2 y_1 y_2, \quad y_3(0) = 1, \quad k^2 = 0.51$$

over the range $[0, 60]$ by using Formula 1 and Formula 2. The largest errors in the last step for various values of h are shown in **Fig. 4** and **Table 4**. The computations were performed in quadruple-precision arithmetic. For comparison, the results obtained by the eleven-stage eighth-order method given by Cooper and Verner[4] are also shown. Figure 4 and Table 4 indicate that all formulas used here are exactly of order eight, because the accumulated truncation errors are proportional to h^8.

Next, to check the stability interval of our formulas, we present the results of an equation[11]:

Example 2: Integrate

$$\frac{dy}{dt} = 100(\sin x - y), \quad y(0) = 0$$

up to 100 steps with various step sizes h. The results are shown in **Table 5**. Quadruple-precision arithmetic was also used. From Table 5, we see that Formula 1 works well for $h \le 0.04$, but that for $h \ge 0.05$ the computation fails. The computation by Formula 2 can be continued for larger values of h than 0.04, but it breaks down for $h \ge 0.07$.

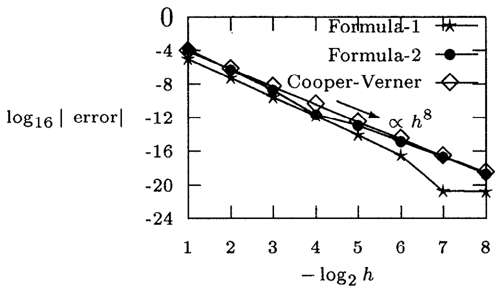

Fig. 4 Largest errors in the numerical solution of Example 1 at the last step.

In this study, we have shown the existence of nine-stage eighth-order limiting formulas, as $c_2 \to 0$ and $c_8 \to c_9 = 1$. The derivatives involved in our formulas are not individual partial derivatives, but the products of the Jacobian matrix and some vector. These products can be calculated very easily by automatic differen-

Table 4 Errors in the numerical solution of Example 1 at the last step.

Step size		Formula 1	Formula 2	Cooper and Verner
2^{-1}	y_1	$.109\times10^{-5}$	$-.238\times10^{-4}$	$-.139\times10^{-4}$
	y_2	$-.759\times10^{-6}$	$.923\times10^{-5}$	$.428\times10^{-5}$
	y_3	$-.281\times10^{-6}$	$.403\times10^{-5}$	$.206\times10^{-5}$
2^{-2}	y_1	$.183\times10^{-8}$	$-.311\times10^{-7}$	$-.357\times10^{-7}$
	y_2	$-.139\times10^{-8}$	$.127\times10^{-7}$	$.115\times10^{-7}$
	y_3	$-.497\times10^{-9}$	$.543\times10^{-8}$	$.560\times10^{-8}$
2^{-3}	y_1	$.332\times10^{-11}$	$-.346\times10^{-10}$	$-.948\times10^{-10}$
	y_2	$-.260\times10^{-11}$	$.148\times10^{-10}$	$.326\times10^{-10}$
	y_3	$-.893\times10^{-12}$	$.634\times10^{-11}$	$.159\times10^{-10}$
2^{-4}	y_1	$.600\times10^{-14}$	$.118\times10^{-13}$	$-.278\times10^{-12}$
	y_2	$-.479\times10^{-14}$	$-.231\times10^{-14}$	$.102\times10^{-12}$
	y_3	$-.151\times10^{-14}$	$-.477\times10^{-15}$	$.496\times10^{-13}$
2^{-5}	y_1	$.100\times10^{-16}$	$.312\times10^{-15}$	$-.902\times10^{-15}$
	y_2	$-.831\times10^{-17}$	$-.119\times10^{-15}$	$.345\times10^{-15}$
	y_3	$-.206\times10^{-17}$	$-.476\times10^{-16}$	$.169\times10^{-15}$

Table 5 Relative errors in numerical solution of Example 2 (E_1: first step, E_{100}: last step).

Step size		Formula 1	Formula 2	Cooper and Verner
0.02	E_1	$-.365\times10^{-3}$	$.270\times10^{-3}$	$.134\times10^{-2}$
	E_{100}	$.391\times10^{-9}$	$-.190\times10^{-9}$	$-.339\times10^{-6}$
0.03	E_1	$-.952\times10^{-2}$	$.401\times10^{-2}$	$.271\times10^{-1}$
	E_{100}	$.239\times10^{-6}$	$-.768\times10^{-7}$	$-.155\times10^{-4}$
0.04	E_1	$-.997\times10^{-1}$	$.227\times10^{-1}$	.238
	E_{100}	$-.383\times10^{-6}$	$.991\times10^{-7}$	$-.557\times10^{-3}$
0.05	E_1	−.626	$.613\times10^{-1}$	1.331
	E_{100}	$-.644\times10^{38}$	$-.110\times10^{-6}$	$-.578\times10^{71}$
0.06	E_1	−2.826	$.141\times10^{-1}$	5.589
	E_{100}	—	$.367\times10^{-9}$	—
0.07	E_1	—	−.658	—
	E_{100}	—	$.632\times10^{58}$	—

tiation, using the intermediate values obtained during the function evaluation. Thus the total cost is about twice the number of intermediate variables and in general is far less than the function evaluation. Moreover, since automatic methods for simultaneous computation of functions and partial derivatives are now available[1),6),15)], our methods can be easily calculated.

In conclusion, we can state that Formula 1 is efficient for non-stiff problems. Simple parameters are preferred, because explicit Runge–Kutta formulas are not suitable for stiff systems.

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Appendix: Outline of the Derivation of Eqs. (29), (30) and a_{54}

Using the notation ρ_i, we see that Eqs. (12), (13), (14), (16), and (20) can be written in the form

$$\sum_{i=4}^{8} \rho_i c_i^k = \frac{1}{\prod_{m=1}^{2}(k+m)} \quad (k=2,3,\cdots,6).$$

From this system, we obtain the solutions ρ_i. By using the last equation of (2) and (6), Eq. (13) can be rewritten in terms of σ_i. From this resultant equation, together with Eqs. (15), (17), and (21), we obtain the system

$$\sum_{i=4}^{7} \sigma_i c_i^k = \frac{1}{\prod_{m=1}^{3}(k+m)} \quad (k=2,3,4,5),$$

and the solutions σ_i.

If all the equations used above hold, then four equations, (19), (24), (25), and (26), can be omitted, as shown below. Replacing σ_i in Eq. (15) with ρ_i in accordance with definition (28), subtracting Eq. (19) from this equation, and substituting $2\sigma_i$ for $\rho_i(1-c_i)$ following from Eq. (29), we see that Eq. (19) becomes Eq. (18). In a very similar way, using Eqs. (17), (19), and (18), we can see that Eqs. (24), (25), and (26) are identical to Eqs. (22), (27), and (23), respectively.

Rewriting c_i^3 in Eq. (15) using the last equation of (2), and then using Eq. (7), together with Eqs. (18) and (22), we obtain

$$\sum_{i=4}^{6} \tau_i c_i^k = \frac{1}{\prod_{m=1}^{4}(k+m)} \quad (k=2,3,4),$$

and the solutions τ_i. Similarly, rewriting Eq. (18) by using the last equation of (2) and (8), together with Eq. (23), we obtain the system

$$\sum_{i=4}^{5} \phi_i c_i^k = \frac{1}{\prod_{m=1}^{5}(k+m)} \quad (k=2,3),$$

and the solutions ϕ_i.

The relation (30) is obtained from Eq. (27) as follows:

(18) $\times\ c_7 -$ (27) yields

$$(\sigma_5(c_7-c_5)a_{54}+\sigma_6(c_7-c_6)a_{64})c_4^3 + \sigma_6(c_7-c_6)a_{65}c_5^3 = \frac{c_7}{840} - \frac{1}{1344}. \quad (39)$$

(15) $\times\ c_7 -$ (17) yields

$$\sigma_4 c_4^3(c_7-c_4)+\sigma_5 c_5^3(c_7-c_5) + \sigma_6 c_6^3(c_7-c_6) = \frac{c_7}{120} - \frac{1}{210}.$$

In the latter equation, rewriting c_i^3 by using the last equation of (2), and then using Eqs. (7) and (9), we obtain

$$(\sigma_5(c_7-c_5)a_{54}+\sigma_6(c_7-c_6)a_{64})c_4^2 + \sigma_6(c_7-c_6)a_{65}c_5^2 = \frac{c_7}{360} - \frac{1}{630}. \quad (40)$$

From the system of Eqs. (39) and (40) we obtain

$$a_{65} = \frac{-56c_4c_7+32c_4+24c_7-15}{20160\sigma_6 c_5^2(c_7-c_6)(c_5-c_4)},$$

while, from Eqs. (28) and (29) we find

$$a_{65} = \frac{\phi_5}{\tau_6} = \frac{5040c_6^2(c_6-c_4)(c_6-c_5)(-8c_4+3)}{20160c_5^2(c_5-c_4)(14c_4c_5-6(c_4+c_5)+3)}.$$

Equating these two values of a_{65}, we get Eq. (30).

The parameter a_{54} in the form shown in the solutions (33) is derived as follows:

From the system of Eqs. (39) and (40), we obtain

$$(\sigma_5(c_7-c_5)a_{54}+\sigma_6(c_7-c_6)a_{64})c_4^2(c_5-c_4) = \frac{56c_5c_7-32c_5-24c_7+15}{20160}, \quad (41)$$

and from Eqs. (28) and (29), we obtain

$$\phi_4 = \tau_4 a_{54} + \tau_5 a_{64} = \frac{8c_5-3}{20160c_4^2(c_5-c_4)}. \quad (42)$$

The solution a_{54} is obtained from the system of Eqs. (41) and (42) as

$$a_{54} = \frac{-c_5^2(c_4(56c_5^2-42c_5+9)-3c_5)}{12c_4^2(14c_4^2-14c_4+3)}$$

and can be written by using Eq. (30) in the form

$$a_{54} = \frac{-54c_4(28c_4^2-21c_4+3)}{(56c_4^2-42c_4+9)^4} = \frac{c_5^3(c_5-c_4)}{c_4^3}.$$

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