学位申請論文

三井斌友

Runge-Kutta Type Integration Formulas Including the Evaluation of the Second Derivative

Part I

Taketomo MITSUI
Research Institute for Mathematical Sciences
Kyoto University, Kyoto.

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Introduction

We are concerning with theoretical study of numerical integration procedure for the initial-value problem of ordinary differential equation:

$$\text{(E)} \qquad \frac{dy}{dx} = f(x,y),$$

$$\text{(IV)} \qquad y(x_I) = y_I.$$

Many numerical analysts have been investigating the discrete variable methods for the problem. Consequently everyone can enjoy to solve ordinary differential equaiton in almost all computing centers. It seems as if we got the numerical integrator through the use of the computer. But the study is yet continued for "better" numerical procedure

Among the one-step methods, Runge-Kutta methods (RK methods, in short) are popular because of the high accuracy and the feasibility of changing step-size. In general the methods are expressed as follows The solution of (E) at x_0+h is approximated by

$$y_1 = y_0 + h \sum_{i=1}^{p} \mu_i k_i,$$

where

$$k_1 = f(x_0, y_0),$$

$$\text{(*)} \qquad k_i = f(x_0 + \alpha_i h, y_0 + h \sum_{j=1}^{i-1} \beta_{ij} k_j), \quad i = 2, \quad ,p,$$

h is the step-size and y_0 is the approximated value at

x_0. This type of the method is called (explicit) p-stage Runge-Kutta algorithm. According to the choice of the stage number p and the parameters α_i, β_{ij}, μ_i we have many variations, among which the classical Runge-Kutta method or the Runge-Kutta-Fehlberg method is famous A distinguished contribution for the study of the Runge-Kutta methods has been made by J C. Butcher ([1] ∿ [4]) He determined the attainable order of the RK methods up to 10-stage formula. On the other hand he introduced the semi-explicit (the summation is up to i instead of i-1 in (*)) or implicit (the summation is up to p in (*)) formula.

RK methods (and perhaps many other quadrature formulas for the initial-value problem) are constructed on the principle that the required function evaluation is only for f(x,y), i.e. the first derivative of the solution. It is quite natural because we are acquainted with the functional form of the first derivative in the ordinary differential equation. Recently, however, some propositions have been made to employ the function evaluation of the second derivative of the solution. Functional form of it is given by

$$g(x,y) = f_x(x,y) + f_y(x,y)f(x,y).$$

M. Urabe [15] made a first attempt to employ g(x,y) by presenting an implicit one-step method with step-size control strategy Let y_0 and y_{-1} be approximations of y(x) at x_0 and x_0-h, respectively His algorithm employs the predictor given by

$$\hat{y}_1 = -31y_{-1} + 32y_0 - h(14f_{-1}+16f_0) + h^2(-2g_{-1}+4g_0)$$

and the corrector given by

$$y_0 = y_{-1} + \frac{h}{240}(101f_{-1} + 128f_0 + 11f_1)$$

$$+ \frac{h^2}{240}(13g_{-1} - 40g_0 - 3\hat{g}_1),$$

where $f_i = f(x_0+ih, y_i)$, $g_i = f(x_0+ih, y_i)$, $\hat{f}_1 = f(x_0+h, y_1)$ and $\hat{g}_1 = g(x_0+h, \hat{y}_1)$ Succeeding his result, J. R. Cash [5] has considered this type of formula more generally and made some stability analysis On the other hand H. Shintani [12], [13] has proposed some formulas analogous to RK formula employing one evaluation for $f(x,y)$ and some for $g(x,y)$ He has given the values of the parameters appearing in the formulas up to the order 7 His results, closely related to the present work, will be mentioned afterward.

In this context another type of integration formula, for the origination of which H. H. Rosenbrook [11] is given credit, is now being developed. It employs the partial derivative $f_y(x,y)$ and is reported to have good stability for stiff systems of ordinary differential equations ([7], [9])

Here we shall examine an explicit (p,q)-stage Runge-Kutta type formula including the second derivative. It requires p times evaluations for the first derivative and q times for the second derivative in a similar manner for RK methods We are interested in the following problems

(1) What is the attainable order of the (p,q)-stage formula from the viewpoint of its local accuracy?

(2) How are the parameters in the formula determined?

(3) What formula is good for practical use?

These problems will be solved in the following sections and the forthcoming paper by the author. The present paper is especially devoted to investigate the (1,q)-stage formulas

First, we shall define explicit (p,q)-stage formula. Next, some algebraic computations are carried out to investigate (p,q)-stage formulas Here SAM software is used as a powerful tool. Then, the attainable order of (1,q)-stage formula is determined up to q=4

Remark. In the case of very complicated functional form of $f(x,y)$ in higher dimension, the calculation of the second derivative $g(x,y)$ requires a laborious work. It is the main reason why the methods employing $g(x,y)$ have not been considered. But the recent development of the symbolic and algebraic manipulation (SAM) software brings the change of the situation. SAM software, for example, REDUCE-2 or MACSYMA, is now a helpful tool for mathematical sciences. In fact, some SAM program may print expressions in a FORTRAN notation so that one can carry out the calculation of the second derivative from $f(x,y)$ in an automatic way Once after algebraic computation we may call $g(x,y)$ as a FUNCTION subprogram.

Moreover, SAM software is very useful for the theoretical study of the RK and its analogous methods For example, H. Toda [14] has considered 5-stage RK limiting formula of order 5. He has utilized MACSYMA essentially We shall also attempt to apply SAM for our study

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§1.1 Explicit (p,q)-Stage Formula

We shall discuss numerical integration procedure for the initial-value problem of ordinary differential equation:

$$\frac{dy}{dx} = f(x,y), \tag{1.1.1}$$

$$y(x_I) = y_I. \tag{1.1.2}$$

Here f is sufficiently smooth with respect to x and y Let us define an explicit (p,q)-stage Runge-Kutta type formula including the second derivative of the solution. Let g stand for the second derivative of $y(x)$,

$$g(x,y) = f_x(x,y) + f_y(x,y)f(x,y) \tag{1.1 3}$$

Explicit (p,q)-stage formula is given as follows

$$y_{n+1} = y_n + h\sum_{i=1}^{p}\mu_i k_i + h^2\sum_{i=1}^{q}\nu_i K_i, \quad n=0,1,2, \tag{1.1 4}$$

where

$$\begin{cases} k_1 = f(x_n+\alpha_1 h,\ y_n), \\ k_i = f(x_n+\alpha_i h,\ y_n+h\sum_{j=1}^{i-1}\beta_{ij}k_j+h^2\sum_{j=1}^{i-1}\gamma_{ij}K_j), \quad i=2,\cdots,p, \end{cases} \tag{1.1.5}$$

$$\begin{cases} K_1 = g(x_n+\rho_1 h,\ y_n+h\sigma_{11}k_1), \\ K_i = g(x_n+\rho_i h,\ y_n+h\sum_{j=1}^{i}\sigma_{ij}k_j+h^2\sum_{j=1}^{i-1}\tau_{ij}K_j), \quad i=2,\cdots,q \end{cases} \tag{1.1.6}$$

Remark 1. The parameters μ_i, ν_i, α_i, β_{ij}, γ_{ij}, ρ_i, σ_{ij} and τ_{ij} are, of course, real numbers

Remark 2. In the case of simultaneous equations in (1), y and f are considered vectors of the same dimension. Then $f_y(x,y)$, the Jacobian matrix of f, is given in the matrix form. For example, assume that

$$f(x,y) = \begin{pmatrix} f_1(y_1,y_2) \\ f_2(y_1,y_2) \end{pmatrix} = \begin{pmatrix} (a_1-b_1y_2)y_1 \\ (a_2-b_2y_1)y_2 \end{pmatrix}$$

where a_i and b_i are constants, then

$$f_y(x,y) = \begin{pmatrix} a_1-b_1y_2 & -b_1y_1 \\ -b_2y_2 & a_2-b_2y_1 \end{pmatrix}$$

and

$$g(x,y) \quad \begin{pmatrix} a_1^2y_1 + (b_2y_1+b_1y_2-2a_1-a_2)b_1y_1y_2 \\ a_2^2y_2 + (b_2y_1+b_1y_2-a_1-2a_2)b_2y_1y_2 \end{pmatrix}$$

Similar to the RK formulas, the determining equations and the parameters are possible to be slightly different between the single differential equation and the systems of equations. For convenience sake we shall investigate the single case The attainable order of the formula is not depend on whether (1) is single or system.

§1.2 The Taylor Series Expansion of the Solution

To investigate Runge-Kutta type methods of higher order, we are required to represent the solution $y(x_0+h)$ for (E) and (IV) in §1 1 into the power series of the stepsize h. For our quadrature formula it is preferable to represent the solution into the power series utilizing the second derivative g.

Twice integration after differentiation for the equation

$$\frac{dy}{dx} = f(x,y), \quad x \geq x_0$$

implies the formula

$$(1.2\ 1) \qquad \int_{x_0}^{x_0+h}\{\int_{x_0}^{t}\frac{d^2y(x)}{dx^2}dx\}dt = \int_{x_0}^{x_0+h}\{\int_{x_0}^{t}g(x,y(x))dx\}dt.$$

The left-hand side of the above formula is equal to

$$y(x_0+h) - y(x_0) - hf(x_0,y(x_0))$$

$$= y(x_0+h) - y_0 - hf_0.$$

Hereafter the subscript 0 stands for the evaluation at $x = x_0$ and $y = y_0$

The right-hand side of (1) becomes

$$\int_0^h\{\int_{x_0}^{x_0+\xi}g(x,y(x))dx\}d\xi = \int_0^h\{\int_0^{\xi}g(x_0+\zeta,\ y(x_0+\zeta))d\zeta\}d\xi$$

Then, assume that for $0 \leq \zeta \leq h$ $y(x_0+\zeta)$ can be expanded in the power series of ζ by

$$(1.2.2) \qquad y(x_0+\zeta) = y_0 + \zeta f_0 + \sum_{r=2}^{m} \frac{\kappa_{r-2}}{r!}\zeta^r + O(\zeta^{m+1}),$$

where κ_j $(j=1,2,\cdots,m)$ is the coefficient to be determined later. Substitution (2) into the integrand implies

$$\begin{aligned} g(x_0+\zeta,y(x_0+\zeta)) &= g(x_0+\zeta,\ y_0+\zeta f_0+\sum_{r=0}^{m}\frac{\kappa_{r-2}}{r!}\zeta^r+O(\zeta^{m+1})) \\ &= \sum_{\ell=0}^{m}\frac{1}{\ell!}[(\zeta\frac{\partial}{\partial x} + (\zeta f_0+\sum_{r=0}^{m}\frac{\kappa_{r-2}}{r!}\zeta^r)\frac{\partial}{\partial y})^{\ell}g]_0 + O(\zeta^{m+1}) \\ &= \sum_{\ell=0}^{m}\frac{\zeta^{\ell}}{\ell!}[(D_0+(\sum_{r=2}^{m}\frac{\kappa_{r-2}}{r!}\zeta^{r-1})\frac{\partial}{\partial y})^{\ell}g]_0 + O(\zeta^{m+1}) \\ &= \sum_{\ell=0}^{m}\frac{\zeta^{\ell}}{\ell!}\{\sum_{k=0}^{\ell}\binom{\ell}{k}(\sum_{r=1}^{m-1}\frac{\kappa_{r-1}}{(r+1)!}\zeta^r)^k \\ &\qquad \times [D_0^{\ell-k}(\frac{\partial}{\partial y})^k g]_0\} + O(\zeta^{m+1}) \end{aligned}$$

Here D_0 is a differential operator defined by

$$D_0 = \frac{\partial}{\partial x} + f_0\frac{\partial}{\partial y}.$$

Therefore we have the following equation:

$$(1.2\ 3) \quad y_0+hf_0+\sum_{r=2}^{m+2}\frac{\kappa_{r-2}}{r!}\zeta^r = y_0+hf_0+$$

$$+\int_0^h(\int_0^{\xi}\sum_{\ell=0}^{m}\frac{\zeta^{\ell}}{\ell!}\{\sum_{k=0}^{\ell}\binom{\ell}{k}(\sum_{r=1}^{m-1}\frac{\kappa_{r-1}}{(r+1)!}\zeta^r)^k[D_0^{\ell-k}(\frac{\partial}{\partial y})g]_0\}d\zeta)d\xi,$$

which determines κ_j recurrently.

Twice differentiation for (3) with respect to h implies

$$(1.2.4)\qquad \sum_{\ell=0}^{m} \frac{\kappa_\ell}{\ell!} h^\ell = \sum_{\ell=0}^{m} \frac{h^\ell}{\ell!} \{ \sum_{k=0}^{\ell} \binom{\ell}{k} \Big(\sum_{r=1}^{m-1} \frac{\kappa_{r-1}}{(r+1)!} h^r \Big)^k \times$$

$$\times [D_0^{\ell-k} (\frac{\partial}{\partial y})^k g]_0 \}$$

Then, we have the following important result.

Theorem 1. The coefficient κ_ℓ $(\ell=0,1,\cdots,m)$ is determined by the following way:

$$(1.2.5)\qquad \begin{cases} \kappa_0 = g_0. \\ \kappa_\ell = [D_0^\ell g]_0 + \sum_{s=1}^{\ell-1} \{ \sum_{t=1}^{m(\ell,s)} \frac{\ell!}{s!(\ell-s-t)!} \times \\ \qquad \times B_{s,t}(\frac{\kappa_0}{2}, \frac{\kappa_1}{3}, \cdots, \frac{\kappa_{s-1}}{s+1}) [D_0^{\ell-s-t} (\frac{\partial}{\partial y})^t g]_0 \}, \\ \qquad\qquad \text{for } \ell=1,2,\cdots,m. \end{cases}$$

Here $B_{s,t}(x_1,x_2,\cdots,x_s)$ is the multivariable polynomial of E. T Bell of the order (s,t) and

$$m(\ell,s) \equiv \min(s,\ell-s)$$

Note. κ_j appeared in the summation of the right-hand side of (5) is for j less than or equal to $\ell-2$ so that we can determine κ_ℓ recurrently by the formula.

Proof $\kappa_0 = g_0$ is clear Let us introduce two

functions $G(h)$ and $A(h;\ell)$ as follows:

$$(1.2.6) \qquad G(h) = \sum_{r=1}^{m-1} \frac{\kappa_{r-1}}{(r+1)!} h^r,$$

$$(1.2.7) \qquad A(h;\ell) \quad \sum_{k=0}^{\ell} \binom{\ell}{k} \{G(h)\}^k [D_0^{\ell-k} (\frac{\partial}{\partial y})^k g]_0, \quad \ell=0,1, \quad ,m.$$

Note that $G(h)$ is of the order h and $G(0) = 0$ holds
Then, the right-hand side of (4) is equal to $\sum_{s=0}^{m} \frac{A(h;s)}{s!} h^s$

Hence, we have the equation

$$(1.2.8) \qquad \sum_{\ell=0}^{m} \frac{\kappa_\ell}{\ell!} h^\ell = \sum_{s=0}^{m} \frac{A(h;s)}{s!} h^s$$

For an integer ℓ such that $1 \leq \ell \leq m$, ℓ-times differentiation to (8) with respect to h implies

$$(1.2.9) \qquad \kappa_\ell = \sum_{s=0}^{\ell-1} \binom{\ell}{s} A^{(s)}(0;\ell-s)$$

By (7), the equation

$$A(0;\ell) = [D_0^\ell g]_0$$

is clear. For $s \geq 1$, we have from (7)

$$\begin{aligned} A^{(s)}(h;\ell-s) = {} & \binom{\ell-s}{1} G^{(s)}(h) [D_0^{\ell-s-1} g_y]_0 + \\ & + \binom{\ell-s}{2} \frac{d^s}{dh^s} \{G(h)\}^2 [D_0^{\ell-s-2} g_{yy}]_0 + \cdots + \\ & + \binom{\ell-s}{k} \frac{d^s}{dh^s} \{G(h)\}^k [D_0^{\ell-s-k} (\frac{\partial}{\partial y})^k g]_0 + \quad + \\ & + \frac{d^s}{dh^s} \{G(h)\}^{\ell-s} [(\frac{\partial}{\partial y})^{\ell-s} g]_0 \end{aligned}$$

For higher derivatives of composite functions, the formula employing the Bell polynomial is known (J Riordan [10]). Hence, applying the formula, we have for $k=1,2,\quad,\ell-s$

$$\frac{d^s}{dh^s}\{G(h)\}^k = \sum_{t=1}^{\min(s,k)} \frac{k!}{(k-t)!} B_{s,t}(G'(h),G''(h),\cdot,G^{(s)}(h))\times \times\{G(h)\}^{k-t},$$

which implies

$$\left[\frac{d^s}{dh^s}\{G(h)\}^k\right]_{h=0} = \begin{cases} k!B_{s,k}(G'(0),G''(0),\cdot,G^{(s)}(0)) & \text{for } s\geq k, \\ 0 & \text{for } s<k. \end{cases}$$

From (6), the equation

$$G^{(s)}(h) = \sum_{r=s}^{m-1} \frac{r!}{(r-s)!}\frac{\kappa_{r-1}}{(r+1)!}h^{r-s} = \sum_{r=s}^{m-1} \frac{\kappa_{r-1}}{(r+1)!(r-s)!}h^{r-s}$$

holds. Hence we have

$$G^{(s)}(0) = \frac{\kappa_{s-1}}{s+1}, \quad s=1,2,\quad,m-1.$$

Then $A^{(s)}(0;\ell-s)$ is given by

$$A^{(s)}(0,\ell-s)=\sum_{k=1}^{m(\ell,s)}\binom{\ell-s}{k}k!B_{s,t}(G'(0),\cdot,G^{(s)}(0))[D_0^{\ell-s-k}(\frac{\partial}{\partial y})^k g]_0$$

$$=\sum_{t=1}^{m(\ell,s)}\frac{(\ell-s)!}{(\ell-s-t)!}B_{s,t}(\frac{\kappa_0}{2},\frac{\kappa_1}{3},\quad,\frac{\kappa_{s-1}}{s+1})[D_0^{\ell-s-t}(\frac{\partial}{\partial y})^t g]_0,$$

which implies from (9)

$$\kappa_\ell = [D_0^\ell g]_0 + \sum_{s=1}^{\ell-1} \binom{\ell}{s} \{ \sum_{t=1}^{m(\ell,s)} \frac{(\ell-s)!}{(\ell-s-t)!} B_{s,t}(\frac{\kappa_0}{2}, \frac{\kappa_1}{3}, \quad , \frac{\kappa_{s-1}}{s+1}) \times$$

$$\times [D_0^{\ell-s-t} (\frac{\partial}{\partial y})^t g]_0 \}$$

$$= [D_0^\ell g]_0 + \sum_{s=1}^{\ell-1} \{ \sum_{t=1}^{m(\ell,s)} \frac{\ell!}{s!(\ell-s-t)!} B_{s,t}(\frac{\kappa_0}{2}, \frac{\kappa_1}{3}. \quad , \frac{\kappa_{s-1}}{s+1}) \times$$

$$\times [D_0^{\ell-s-t} (\frac{\partial}{\partial y})^t g]_0 \}$$

This is the desired result.□

The multivariable polynomial $B_{s,t}(x_1, x_2, \cdot, x_s)$ has a recurrence formula to calculate it conveniently by the application of any SAM software That is,

$$\sum_{t=1}^{s} x_1 B_{s,t}(x_1, \quad , x_s) a^{t+1} + \sum_{t=1}^{s} (\sum_{k=1}^{s} x_{k+1} \frac{\partial B_{s,t}}{\partial x_k}) a^t$$

$$= \sum_{t=1}^{s+1} B_{s+1,t}(x_1, \cdot, x_{s+1}) a^t$$

Here, the both sides of the formula is considered as a polynomial of a. The recurrence formula for $B_{s,t}$ will be employed during the calculations of κ_ℓ by REDUCE-2

Theorem 1 tells us a concrete method to determine the Taylor series expansion (2) employing the second derivative. For example,

$$\kappa_1 = [D_0 g]_0,$$

$$\kappa_2 = [D_0^2 g]_0 + 2!B_{1,1}(\frac{\kappa_0}{2})g_{y,0} = [D_0^2 g]_0 + \kappa_0 g_{y,0}$$

$$= [D_0^2 g]_0 + g_0 g_{y,0},$$

$$\kappa_3 = [D_0^3 g]_0 + 3!B_{1,1}(\frac{\kappa_0}{2})[D_0 g_y]_0 + \frac{3!}{2!}B_{2,1}(\frac{\kappa_0}{2}, \frac{\kappa_1}{3})g_{y,0}$$

$$= [D_0^3 g]_0 + 3\kappa_0[D_0 g_y]_0 + \kappa_1 g_{y,0}$$

$$= [D_0^3 g]_0 + 3g_0[D_0 g_y]_0 + [D_0 g]_0 g_{y,0}.$$

We may also carry out the process by the SAM software up to the desired order. The result by REDUCE-2 is shown in Table 1.

Note that because of Remark 2 in the preceding section we do not care the order of the higher partial derivatives.

Another important result from Theorem 1 is that any κ_j is a summation of an integer multiple of some product of $[D_0^p(\frac{\partial}{\partial y})^q g]_0$ Hence, we shall call any product of $[D_0^p(\frac{\partial}{\partial y})^q g]_0$ an elementary differential of g. J C. Butcher [1] has used the terminology of elementary differential in a different sense However, our study of the expression of the coefficient of Taylor series in the elementary differentials is on the similar point of view.

In fact, the way of the proof of Theorem 1 is applicable to the Taylor series expansion of $y(x_0+h)$ employing the first derivative.

Theorem 2 Assume that

$$(1.2.10) \qquad y(x_0+h) = y_0 + \sum_{r=1}^{m} \frac{\lambda_{r-1}}{r!}h^r + O(h^{m+1}).$$

Then, the coefficient λ_ℓ $(\ell=0,1,\cdots,m-1)$ is determined by

$$(1.2.11) \quad \begin{cases} \lambda_0 = f_0 \\ \lambda_\ell = [D_0^\ell f]_0 + \sum_{s=1}^{\ell-1} \left(\sum_{t=1}^{m(\ell,s)} \frac{\ell!}{(\ell-s-t)!s!} \times \right. \\ \qquad \left. \times B_{s,t}\left(\frac{\lambda_1}{2}, \frac{\lambda_2}{3}, \quad , \frac{\lambda_s}{s+1}\right)[D_0^{\ell-s-t}\left(\frac{\partial}{\partial y}\right)^t f]_0 \right\}, \\ \qquad\qquad\qquad\qquad \ell=1,2, \quad ,m. \end{cases}$$

We shall call (10) the first type power series expansion in contrast with (2) which will be mentioned as the second type expansion.

Table 1

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§1.3 Implicit (1,q)-Stage Formula.

For the study of the general (1,q)-stage formula, it is convenient to analyse the corresponding implicit (1,q)-stage formula, because we gain an insight into its algebraic relations by them.

Consider an implicit (1,q)-stage formula as follows:

$$(1\ 3.1)\quad y_{n+1} = y_n + \mu_1 h k_1 + \sum_{i=1}^{q} \nu_i h^2 K_i, \quad n = 0, 1, 2, \cdots,$$

$$(1.3.2)\quad \begin{cases} k_1 = f(x_n+\alpha_1 h,\ y_0), \\ K_i = g(x_n+\rho_i h,\ y_n+\sigma_{i1} h k_1 + \sum_{j=1}^{q} \tau_{ij} h^2 K_j), \quad i = 1, \cdot, q. \end{cases}$$

We need to analyse one-step integration by (1) and (2), so we may substitute n=0, i e.

$$(1.3.3)\quad \begin{cases} y_1 = y_0 + \mu_1 h k_1 + \sum_{i=1}^{q} \nu_i h^2 K_i, \\ k_1 = f(x_0 + \alpha_1 h,\ y_0), \\ K_i = g(x_0 + \rho_i h,\ y_0 + \sigma_{i1} h k_1 + \sum_{j} \tau_{ij} h^2 K_j), \quad i = 1, \cdot, q \end{cases}$$

For k_1, we have the following expansion:

$$k_1 = f_0 + \alpha_1 h\, f_{x,0} + \frac{1}{2}\alpha_1^2 h^2 f_{xx,0} + O(h^3)$$

On the other hand, K_i has the expansion

$$K_i = g_o + O(h)$$

Hence, the equation

$$(1.3\ 4)\quad y_1 = y_0 + \mu_1 h f_0 + h^2(\mu_1\alpha_1 f_{x,0} + \sum_{i=1}^{q} \nu_i g_0) + O(h^3)$$

holds The solution $y(x_0+h)$ has the power series of h as follows:

$$(1.3.5)\quad y(x_0+h) = y_0 + hf_0 + \frac{1}{2} h^2 g_0 + O(h^3)$$

Comparison of the terms having the same power of h in (4) and (5) yields the following equations.

$$\mu_1 = 1,$$

$$\mu_1\alpha_1 f_{x,0} + \sum_{i=1}^{q} \nu_i g_0 = \frac{1}{2} g_0.$$

Thus, $\mu_1=1$, $\alpha_1=0$ and $\sum_{i=1}^{q} \nu_i=\frac{1}{2}$ must hold in the implicit (1,q)-stage formula.

Next, since K_i has the expansion

$$K_i = g_0 + [(\rho_i\frac{\partial}{\partial x} + \sigma_{i1} f_0 \frac{\partial}{\partial y})g]_0 h + O(h^2),$$

the comparison of the third order term of y_1 and $y(x_0+h)$ implies the equation.

$$\frac{1}{2}[D_0 g]_0 = \frac{1}{2}(g_{x,0} + f_0 \cdot g_{y,0}) = \sum_{i=1}^{q} \nu_i [(\rho_i g_{x,0} + \sigma_{i1} f_0 \cdot g_{y,0})]$$

From the viewpoint of homogenuity of differential operation, $\rho_i = \sigma_{i1}$ must hold for $i=1,2, \cdot, q$

Hence, let us rewrite (3) by

$$(1.3.6) \quad \begin{cases} y_1 = y_0 + hf_0 + \sum_{i=1}^{q} \nu_i h^2 k_i, \\ K_i = g(x_0+\rho_i h,\ y_0+\rho_i h f_0+\sum_j \tau_{ij} h^2 K_j), \quad i = 1, \cdot\cdot, q \end{cases}$$

We shall assume the Taylor series expansion for K_i by

$$(1.3.7) \qquad K_i = \sum_{\ell=0}^{m} \frac{\kappa_{i\ell}}{\ell!} h^{\ell} + O(h^{m+1}),$$

where $\kappa_{i\ell}$ will be determined by the similar manner for Theorem 1.

Theorem 3. For each i, $\kappa_{i\ell}$ in (1.3.7) is determined by the following:

$$(1\ 3.8) \quad \begin{cases} \kappa_{i0} = g_0, \\ \kappa_{i\ell} = \rho_i^{\ell}[D_0^{\ell} g]_0 + \sum_{s=1}^{\ell-1} \left\{ \sum_{t=1}^{m(\ell,s)} \frac{\ell!}{s!(\ell-s-t)!} \rho_i^{\ell-s-t} \right. \\ \qquad \times B_{s,t}\left(\sum_{j=1}^{q} \tau_{ij}\kappa_{j0}, \quad , s\sum_j \tau_{ij}\kappa_{j,s-1}\right) \\ \qquad \left. \times [D_0^{\ell-s-t}(\frac{\partial}{\partial y})^t g]_0 \right\}, \quad \ell = 1, 2, \quad , m. \end{cases}$$

Note. By the above formula, $\kappa_{i\ell}$ can be determined in the ascending order of the second subscript, i.e., κ_{i2} $(i=1,\cdots,q)$ after κ_{i1}, κ_{i3} $(i=1,\cdots,q)$ after κ_{i2}, and so on.

Proof. Two-variable Taylor series expansion for K_i gives

$$K_i = \sum_{\ell=0}^{m} \frac{1}{\ell!}[\{\rho_i h\frac{\partial}{\partial x} + (\rho_i h f_0 + \sum \tau_{ij} h^2 K_j)\frac{\partial}{\partial y}\}^{\ell} g]_0 + O(h^{m+1})$$

$$= \sum_{\ell=0}^{m} \frac{h^{\ell}}{\ell!}[\{\rho_i D_0 + (\sum \tau_{ij} h K_j)\frac{\partial}{\partial y}\}^{\ell} g]_0 + O(h^{m+1})$$

$$= \sum_{\ell=0}^{m} \frac{h^{\ell}}{\ell!}[\{\rho_i D_0 + (\sum_{r=0}^{m-1}(\sum_{j=1}^{q} \frac{\tau_{ij}\kappa_{jr}}{r!})h^{r+1})\frac{\partial}{\partial y}\}^{\ell} g]_0 + O(h^{m+1})$$

$$= \sum_{\ell=0}^{m} \frac{h^{\ell}}{\ell!}\{\sum_{k=0}^{\ell} \binom{\ell}{k} \rho_i^{\ell-k} (\sum_{r=0}^{m-1}(\sum_{j} \frac{\tau_{ij}\kappa_{jr}}{r!})h^{r+1})^k [D_0^{\ell-k}(\frac{\partial}{\partial y})^k g]_0\} + O(h^{m+1})$$

Thus, putting $G_i(h)$ as

$$G_i(h) = \sum_{r=0}^{m-1}(\sum_{j=1}^{q} \frac{\tau_{ij}\kappa_{jr}}{r!})h^{r+1} \tag{1.3.9}$$

and noting that $G_i(h)$ is of the order h and $G_i(0)=0$, we have the equation

$$\sum_{\ell=0}^{m} \frac{\kappa_{i\ell}}{\ell!} h^{\ell} = \sum_{\ell=0}^{m} \frac{h^{\ell}}{\ell!}\{\sum_{k=0}^{\ell} \binom{\ell}{k} \rho_i^{\ell-k} (G_i(h))^k [D_0^{\ell-k}(\frac{\partial}{\partial y})^k g]_0\} ,$$

which is similar to (1.2 4) Hence, following after the proof of Theorem 1, we have

$$\kappa_{i\ell}=\rho_i^{\ell}[D_0^{\ell}g]_0+\sum_{s=1}^{\ell-1}\binom{\ell}{s}\{\sum_{t=1}^{m(\ell,s)}\frac{(\ell-s)!}{(\ell-s-t)!}\rho_i^{\ell-s-t}B_{s,t}(G_i'(0),\quad ,G_i^{(s)}(0))$$

$$\times[D_0^{\ell-s-t}(\frac{\partial}{\partial y})^t g]_0\}$$

From (9), for $k=1,2,\quad ,s$

$$G_i^{(k)}(h)=\sum_{r=k-1}^{m-1}\frac{(r+1)!}{(r-k+1)!}(\sum_j\frac{\tau_{ij}\kappa_{jr}}{r!})h^{r-k+1}$$

holds, which implies

$$G_i^{(k)}(0)=k!(\sum_j\frac{\tau_{ij}\kappa_{j,k-1}}{(k-1)!})=k\sum_j\tau_{ij}\kappa_{j,k-1}$$

Thus we have the desired result. □

By Theorem 3, $\kappa_{i\ell}$ is given as follows:

$$\kappa_{i1}=\rho_i[D_0g]_0,$$

$$\kappa_{i2}=\rho_i^2[D_0^2g]_0+2!B_{1,1}(\sum_j\tau_{ij}\kappa_{j0})\,g_{y,0}$$

$$=\rho_i^2[D_0^2g]_0+2(\sum_j\tau_{ij})g_0\,g_{y.0}\ ,$$

$$\kappa_{i3}=\rho_i^3[D_0^3g]_0+3!\rho_i\,B_{1,1}(\sum\tau_{ij}\kappa_{j0})[D_0g_y]_0+3B_{2,1}(\sum\tau_{ij}\kappa_{j0},2\sum\tau_{ij}\kappa_{j1})\cdot g_y$$

$$=\rho_i^3[D_0^3g]_0+6\rho_i(\sum_j\tau_{ij})g_0\,[D_0g_y]_0+6(\sum_j\tau_{ij}\rho_j)[D_0g]_0\,g_{y,0}$$

The result with the help of REDUCE-2 is shown in Table 2
Here we employ the notation

$$T_{ik} = \sum_{j=1}^{q} \rho_j^k \tau_{ij} \ , \quad i = 1, 2, \quad , q, \ k = 0, 1, 2, \cdot$$

From (6) and (7), the Taylor series expansion for y_1 is given by

$$(1.3.10) \quad y_1 = y_0 + hf_0 + \sum_{i=1}^{q} \nu_i h^2 \Big(\sum_{\ell=0}^{m} \frac{\kappa_{i\ell}}{\ell!} h^{\ell} \Big) + O(h^{m+3})$$

$$= y_0 + hf_0 + \sum_{\ell=0}^{m} \Big(\sum_{i=1}^{q} \nu_i \kappa_{i\ell} \Big) \frac{h^{\ell+2}}{\ell!} + O(h^{m+3})$$

$$= y_0 + hf_0 + \sum_{r=2}^{m} \Big(\sum_{i=1}^{q} \nu_i \kappa_{i,r-2} \Big) \frac{h^r}{(r-2)!} + O(h^{m+1})$$

On the other hand, from (1.2 2), the (second type) Taylor series expansion of the solution $y(x_0+h)$ is given by

$$(1.3.11) \quad y(x_0+h) = y_0 + hf_0 + \sum_{r=2}^{m} \frac{\kappa_{r-2}}{r!} h^r + O(h^{m+1}),$$

where κ_ℓ is represented by (1.2 5) The comparison of (10) and (11) brings the determining equation of the implicit (1,q)-stage formula, for which we have the following

Theorem 4 Each $\kappa_{i\ell}$ in (10) is constructed with the all elementary differentials included in the corresponding κ_ℓ in (11) Hence the determining equation of the implicit

(1,q)-stage formula is of the form such as

(an integer) × (a polynomial of ν_i, ρ_i, τ_{ij}) = (an integer).

Proof From (10) and (11), κ_ℓ and $\kappa_{i,\ell}$ must satisfy

$$\frac{1}{\ell!}\sum_{i=1}^{q}\nu_i\kappa_{i\ell} = \frac{\kappa_\ell}{(\ell+2)!}, \quad \ell = 0, 1, 2, \quad , m-2,$$

which implies

$$(\ell+1)(\ell+2)\sum_{i}\nu_i\kappa_{i\ell} = \kappa_\ell$$

From (1.2 5) and (1.3.8) the conclusion follows □

Table 2

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§1.4 Determining Equation for (1,q)-Stage Formula.

An algebraic computation according to Theorem 1 gives the number of elementary differentials including in each κ_ℓ. Let m_ℓ be the number of elementary differentials in κ_ℓ and define the integer M_ℓ by

$$M_\ell = \sum_{j=0}^{\ell} m_j$$

Each m_ℓ and M_ℓ are given in Table 3 up to $\ell = 8$.

Thus, we have M_ℓ restrictions for the parameters ν_i, ρ_i, τ_{ij} of the formula. In the implicit (1,q)-stage formula the number of the parameters to be determined, say $N_q^{(I)}$, can be given as a simple function of q

$$N_q^{(I)} = q(q+2)$$

It implies that the implicit (1,q)-stage formula can attain at least the order $(\bar{\ell}+2)$ where $\bar{\ell}$ is the largest integer satisfying the inequality $M_\ell \leq N_q^{(I)}$ These relations are shown in Table 4

However, the above argument based on merely counting the number of the equations that must be satisfied, ignores the relationship between them. In fact, it may happen that M_ℓ restrictions are satisfied with fewer than M_ℓ variables. But, since we are interested in the explicit formula rather than implicit one, we shall not come into more investigation

for the attainable order of the implicit formula.

An explicit (1,q)-stage formula, which is defined by the parameters ν_i, ρ_i and τ_{ij} ($\tau_{ij} = 0$ for $j \geq i$) in (1.3.6), has $N_q^{(E)}$ parameters to be determined. Here $N_q^{(E)}$ is given by

$$N_q^{(E)} = q(q+3)/2.$$

Hence, similar consideration for the implicit case gives the largest integer ℓ^* satisfying the inequality $M_\ell \leq N_q^{(E)}$. Table 4 includes the relations between q, the number of stages, and ℓ^*

Table 3.

ℓ	m_ℓ	M_ℓ
0	1	1
1	1	2
2	2	4
3	3	7
4	6	13
5	9	22
6	17	39
7	26	65
8	46	111

Table 4.

q	$N_q^{(I)}$	$\bar{\ell}$	$N_q^{(E)}$	ℓ^*
1	3	1	2	1
2	8	3	5	2
3	15	4	9	3
4	24	5	14	4
5	35	5	20	5
6	48	6	27	5
7	63	6	35	6
8	80	7	44	6
9	99	7	54	6
10	120	8	65	7

Shintani has given some explicit one-step methods utilizing the second derivative [12], whose formulation coincides with our explicit (1,q)-stage formula. He has determined the parameters for $q = 1, 2, 3, 4$ and 5 which give the formula obtaining the order $3, 4, 5, 6$ and 7 respectively His results attain the orders that we have argued as the least number ℓ^* for each stage formula. Hence, it is a question whether Shintani's results can be improved.

We shall consider the determining equation for the explicit (1,q)-stage formula. Tables 1 and 2 give the equation as follows. We employ the notation for summation symbol such that the upper limit of summation can not exceed the variable of the preceding summation symbols, i.e. $\sum_{i} \cdots (\sum_{j} \cdots)$ means $\sum_{i=1}^{q} \cdots (\sum_{j=1}^{i-1} \cdots)$ Moreover, the symbol T_{ik} means

$$T_{1k} = 0 \quad \text{and} \quad T_{ik} = \sum_{j=1}^{i-1} \rho_i^k \tau_{ij}, \quad i = 2,3, \quad ,q.$$

Determining equations.

$\ell = 0$: (E-0) $\quad 2\sum_i \nu_i = 1$

$\ell = 1$: (E-1) $\quad 6\sum_i \nu_i \rho_i - 1$

$\ell = 2$: (E-21) $\quad 12\sum_i \nu_i \rho_i^2 - 1$

(E-22) $\quad 24\sum_i \nu_i T_{i0} - 1$

$\ell = 3$: (E-31) $\quad 20\sum_i \nu_i \rho_i^3 = 1$

(E-32) $\quad 120\sum_i \nu_i T_{i1} = 1$

(E-33) $\quad 120\sum_i \nu_i \rho_i T_{i0} = 3$

$\ell = 4$: (E-41) $\quad 30\sum_i \nu_i \rho_i^4 = 1$

(E-42) $\quad 360\sum_i \nu_i T_{i_2} = 1$

(E-43) $\quad 720\sum_i \nu_i \rho_i T_{i1} = 4$

(E-44) $\quad 360\sum_i \nu_i \rho_i^2 T_{i0} = 6$

(E-45) $\quad 720\sum_i \sum_j \nu_i \tau_{ij} T_{j0} = 1$

(E-46) $\quad 360\sum_i \nu_i T_{i0}^2 = 3$

$\ell = 5$: (E-51) $42\sum_i \nu_i \rho_i^5 = 1$

(E-52) $840\sum_i \nu_i T_{i3} = 1$

(E-53) $2520\sum_i \nu_i \rho_i T_{i2} = 5$

(E-54) $2520\sum_i \nu_i \rho_i^2 T_{i1} = 10$

(E-55) $5040\sum_i \sum_j \nu_i \tau_{ij} T_{j1} = 1$

(E-56) $840\sum_i \nu_i \rho_i^3 T_{i0} = 10$

(E-57) $5040\sum_i \sum_j \nu_i (\rho_i + \rho_j) \tau_{ij} T_{j0} = 8$

(E-58) $5040\sum_i \nu_i T_{i0} T_{i1} = 10$

(E-59) $2520\sum_i \nu_i \rho_i T_{i0}^2 = 15$

$\ell = 6$: (E-601) $56\sum_i \nu_i \rho_i^6 = 1$

(E-602) $1680\sum_i \nu_i T_{i4} = 1$

(E-603) $6720\sum_i \nu_i \rho_i T_{i3} = 6$

(E-604) $10080\sum_i \nu_i \rho_i^2 T_{i2} = 15$

(E-605) $20160\sum_i \sum_j \nu_i \tau_{ij} T_{j2} = 1$

(E-606) $6720\sum_i \nu_i \rho_i^3 T_{i1} = 20$

(E-607) $40320\sum_i \sum_j \nu_i (\rho_i+\rho_j)\tau_{ij} T_{j1} = 10$

(E-608) $20160\sum_i \nu_i T_{i1}^2 - 10$

(E-609) $1680\sum_i \nu_i \rho_i^4 T_{i0} = 15$

(E-610) $40320\sum_i \sum_j \nu_i \rho_i \rho_j \tau_{ij} T_{j0} = 18$

(E-611) $20160\sum_i \sum_j \nu_i (\rho_i^2+\rho_j^2)\tau_{ij} T_{j0} = 21$

(E-612) $40320\sum_i \sum_j \sum_k \nu_i \tau_{ij} \tau_{jk} T_{k0} = 1$

(E-613) $20160\sum_i \nu_i T_{i0} T_{i2} = 15$

(E-614) $40320\sum_i \nu_i \rho_i T_{i0} T_{i1} = 60$

(E-615) $10080\sum_i \nu_i \rho_i^2 T_{i0}^2 = 45$

(E-616) $20160\sum_i \sum_j \nu_i \tau_{ij} (T_{j0}+2T_{i0}) T_{j0} = 18$

(E-617) $6720\sum_i \nu_i T_{i0}^3 = 15$

$\ell = 7$: (E-701) $\frac{1}{11}72\sum_i \nu_i \rho_i^7 = 1$

(E-702) $3024\sum_i \nu_i T_{i5} = 1$

(E-703) $$15120\sum_i \nu_i \rho_i T_{i4} = 7$$

(E-704) $$30240\sum_i \nu_i \rho_i^2 T_{i3} = 21$$

(E-705) $$60480\sum_i \sum_j \nu_i \tau_{ij} T_{j3} = 1$$

(E-706) $$30240\sum_i \nu_i \rho_i^3 T_{i2} = 35$$

(E-707) $$181440\sum_i \sum_j \nu_i (\rho_i+\rho_j) \tau_{ij} T_{j2} = 12$$

(E-708) $$15120\sum_i \nu_i \rho_i^4 T_{i1} = 35$$

(E-709) $$362880\sum_i \sum_j \nu_i \rho_i \rho_j \tau_{ij} T_{j1} = 28$$

(E-710) $$181440\sum_i \sum_j \nu_i (\rho_i^2+\rho_j^2) \tau_{ij} T_{j1} = 31$$

(E-711) $$362880\sum_i \sum_j \sum_k \nu_i \tau_{ij} \tau_{jk} T_{k1} = 1$$

(E-712) $$181440\sum_i \nu_i T_{i1} T_{i2} = 35$$

(E-713) $$181440\sum_i \nu_i \rho_i T_{i1}^2 = 70$$

(E-714) $$3024\sum_i \nu_i \rho_i^5 T_{i0} = 21$$

(E-715) $$181440\sum_i \sum_j \nu_i \rho_i \rho_j (\rho_i+\rho_j) \tau_{ij} T_{j0} = 105$$

(E-716) $$60480\sum_i \sum_j \nu_i (\rho_i^3+\rho_j^3) \tau_{ij} T_{j0} = 45$$

(E-717) $362880\sum_i\sum_j\sum_k \nu_i(\rho_i+\rho_j+\rho_k)\tau_{ij}\tau_{jk}T_{k0} = 15$

(E-718) $60480\sum_i \nu_i T_{i0}T_{i3} = 21$

(E-719) $181440\sum_i \nu_i \rho_i T_{i0}T_{i2} = 105$

(E-720) $181440\sum_i \nu_i \rho_i^2 T_{i0}T_{i1} = 210$

(E-722) $362880\sum_i\sum_j \nu_i\tau_{ij}(T_{i0}T_{j1}+T_{j0}T_{j1}+T_{j0}T_{i1}) = 66$

(E-723) $30240\sum_i \nu_i \rho_i^3 T_{i0}^2 = 105$

(E-724) $181440\sum_i\sum_j \nu_i(2\rho_i T_{i0}+\rho_j T_{j0})\tau_{ij}T_{j0} = 84$

(E-725) $181440\sum_i\sum_j \nu_i(\rho_i T_{j0}+2\rho_j T_{i0})\tau_{ij}T_{j0} = 120$

(E-726) $181440\sum_i \nu_i T_{i0}^2 T_{i1} = 105$

(E-727) $60480\sum_i \nu_i \rho_i T_{i0}^3 = 105$

$\ell = 8$: (E-801) $90\sum_i \nu_i \rho_i^8 = 1$

(E-802) $5040\sum_i \nu_i T_{i6} = 1$

(E-803) $30240\sum_i \nu_i \rho_i T_{i5} = 8$

(E-804) $75600\sum_i \nu_i \rho_i^2 T_{i4} = 28$

(E-805) $$151200\sum_i\sum_j \nu_i\tau_{ij}T_{j4} = 1$$

(E-806) $$100800\sum_i \nu_i\rho_i^3T_{i3} = 56$$

(E-807) $$604800\sum_i\sum_j \nu_i(\rho_i+\rho_j)\tau_{ij}T_{j3} = 14$$

(E-808) $$75600\sum_i \nu_i\rho_i^4T_{i2} = 70$$

(E-809) $$1814400\sum_i\sum_j \nu_i\rho_i\rho_j\tau_{ij}T_{j2} = 40$$

(E-810) $$907200\sum_i\sum_j \nu_i(\rho_i^2+\rho_j^2)\tau_{ij}T_{j2} = 43$$

(E-811) $$1814400\sum_i\sum_j\sum_k \nu_i\tau_{ij}\tau_{jk}T_{k2} = 1$$

(E-812) $$453600\sum_i \nu_i T_{i2}^2 = 35$$

(E-813) $$30240\sum_i \nu_i\rho_i^5T_{i1} = 56$$

(E-814) $$1814400\sum_i\sum_j \nu_i\rho_i\rho_j(\rho_i+\rho_j)\tau_{ij}T_{j1} = 192$$

(E-815) $$604800\sum_i\sum_j \nu_i(\rho_i^3+\rho_j^3)\tau_{ij}T_{ji} = 76$$

(E-816) $$3628800\sum_i\sum_j\sum_k \nu_i(\rho_i+\rho_j+\rho_k)\tau_{ij}\tau_{jk}T_{k1} = 18$$

(E-817) $$604800\sum_i \nu_i T_{i1}T_{i3} = 56$$

(E-818) $$1814400\sum_i \nu_i\rho_i T_{i1}T_{i2} = 280$$

(E-819) $907200\sum_i \nu_i \rho_i^2 T_{i1}^2 = 280$

(E-820) $1814400\sum_i \sum_j \nu_i \tau_{ij} T_{j1}(2T_{i1}+T_{j1}) = 66$

(E-821) $5040\sum_i \nu_i \rho_i^6 T_{i0} = 28$

(E-822) $907200\sum_i \sum_j \nu_i \rho_i^2 \rho_j^2 \tau_{ij} T_{j0} = 168$

(E-823) $604800\sum_i \sum_j \nu_i \rho_i \rho_j (\rho_i^2+\rho_j^2) \tau_{ij} T_{j0} = 248$

(E-824) $151200\sum_i \sum_j \nu_i (\rho_i^4+\rho_j^4) \tau_{ij} T_{j0} = 85$

(E-825) $3628800\sum_i \sum_j \sum_k \nu_i (\rho_i \rho_j+\rho_j \rho_k+\rho_j \rho_k) \tau_{ij} \tau_{jk} T_{k0} = 82$

(E-826) $1814400\sum_i \sum_j \sum_k \nu_i (\rho_i^2+\rho_j^2+\rho_k^2) \tau_{ij} \tau_{jk} T_{k0} = 49$

(E-827) $3628800\sum_i \sum_j \sum_k \sum_\ell \nu_i \tau_{ij} \tau_{jk} \tau_{k\ell} T_{\ell 0} = 1$

(E-828) $151200\sum_i \nu_i T_{i0} T_{i4} = 28$

(E-829) $604800\sum_i \nu_i \rho_i T_{i0} T_{i3} = 168$

(E-830) $907200\sum_i \nu_i \rho_i^2 T_{i0} T_{i2} = 420$

(E-831) $1814400\sum_i \sum_j \nu_i \tau_{ij} (T_{i2} T_{j0}+T_{i0} T_{j2}+T_{j0} T_{j2}) = 113$

(E-832) $604800\sum_i \nu_i \rho_i^3 T_{i0} T_{i1}$ 560

(E-833) $3628800\sum_i\sum_j \nu_i\tau_{ij}(\rho_j T_{i0}T_{j1}+\rho_j T_{i1}T_{j0}+\rho_i T_{j0}T_{j1}) = 360$

(E-834) $3628800\sum_i\sum_j \nu_i\tau_{ij}(\rho_i T_{i0}T_{j1}+\rho_i T_{i1}T_{j0}+\rho_j T_{j0}T_{j1}) = 508$

(E-835) $1814400\sum_i \nu_i T_{i0}T_{i1}^2 = 280$

(E-836) $75600\sum_i \nu_i \rho_i^4 T_{i0}^2 = 210$

(E-837) $907200\sum_i\sum_j \nu_i\tau_{ij}(\rho_i^2 T_{j0}+2\rho_j^2 T_{i0})T_{j0} = 252$

(E-838) $1814400\sum_i\sum_j \nu_i\rho_i\rho_j\tau_{ij}(2T_{i0}+T_{j0})T_{j0} = 624$

(E-839) $907200\sum_i\sum_j \nu_i\tau_{ij}(\rho_j^2 T_{j0}+2\rho_i^2 T_{i0})T_{j0} = 465$

(E-840) $1814400\sum_i\sum_j\sum_k \nu_i\tau_{ij}(2\tau_{jk}T_{i0}T_{k0}+2\tau_{jk}T_{j0}T_{k0}+\tau_{ik}T_{j0}T_{k0}+\tau_{jk}T_{k0}^2) - 81$

(E-841) $907200\sum_i \nu_i T_{i0}^2 T_{i2} = 210$

(E-842) $1814400\sum_i \nu_i \rho_i T_{i0}^2 T_{i1} = 840$

(E-843) $302400\sum_i \nu_i \rho_i^2 T_{i0}^3 = 420$

(E-844) $1814400\sum_i\sum_j \nu_i\tau_{ij}T_{i0}T_{j0}^2 = 84$

(E-845) $604800\sum_i\sum_j \nu_i\tau_{ij}(3T_{i0}^2+T_{j0}^2)T_{j0}$ 225

(E-846) $151200\sum_i \nu_i T_{i0}^4 = 105$

§1.5 Attainable Order of (1,1)- and (1,2)-Stage Formulas

The explicit (1,q)-stage formula is said to have the attainable order m if m is the largest integer for which

$$y(x+h) - y_1 = O(h^{m+1})$$

among all combinations of the parameters of the formula, where $y(x)$ is the analytical solution and y_1 is given by (1.3 6) The definition of the attainable order will be extended, if necessary, to general (p,q)-stage formula.

It is obvious that a (1,q)-stage formula has the attainable order m if and only if the determining equations corresponding up to ℓ have at least one solution, but they have no solution up to $\ell+1$, where $\ell = m-2$.

Theorem 5. The attainable order of (1,1)-stage formula is 3

Proof The left-hand side of the equation (E-22) is equal to

$$24 \sum_i \nu_i (\sum_j \tau_{ij}),$$

which vanishes for (1,1)-stage formula because $\sum_j \tau_{ij} = 0$ This means that the parameters ν_1 and ρ_1 can satisfy merely the equations (E-0) and (E-1) □

Theorem 6. The attainable order of (1,2)-stage formula is equal to 4.

Proof Assume that the formula attains order 5, that is, the parameters ν_1, ν_2, ρ_1, ρ_2 and τ_{21} satisfy the equations (E-0) $\sim$ (E-33).

(1.5.1) $\quad \nu_1 + \nu_2 = \frac{1}{2}$

(1 5.2) $\quad \nu_1\rho_1 + \nu_2\rho_2 = \frac{1}{6}$

(1 5.3) $\quad \nu_2\tau_{21} = \frac{1}{24}$

(1 5 4) $\quad \nu_1\rho_1^2 + \nu_2\rho_2^2 = \frac{1}{12}$

(1.5.5) $\quad \nu_2\rho_2\tau_{21} = \frac{1}{40}$

(1 5.6) $\quad \nu_2\rho_1\tau_{21} = \frac{1}{120}$

(1 5 7) $\quad \nu_1\rho_1^3 + \nu_2\rho_2^3 = \frac{1}{20}$

The equations (1), (2) and (4) yield a matrix equation

$$\begin{pmatrix} 1 & 1 & 1/2 \\ \rho_1 & \rho_2 & 1/6 \\ \rho_1^2 & \rho_2^2 & 1/12 \end{pmatrix} \begin{pmatrix} \nu_1 \\ \nu_2 \\ -1 \end{pmatrix} = 0,$$

which implies

$$(1.5.8)\qquad \begin{vmatrix} 1 & 1 & 1/2 \\ \rho_1 & \rho_2 & 1/6 \\ \rho_1^2 & \rho_2^2 & 1/12 \end{vmatrix} = 0$$

for the existence of nontrivial solution $[\nu_1, \nu_2, -1]^t$
On the other hand, (3), (5) and (6) give the values

$$\rho_1 = \frac{1}{5}, \qquad \rho_2 = \frac{3}{5},$$

which specify the determinant of (8) by $\frac{1}{250}$. This contradiction implies the statement □

Note. Shintani gives (1,1)-stage formula with parameters $\nu_1 = \frac{1}{2}$ and $\rho_1 = \frac{1}{3}$. He also gives (1,2)-stage formula with $\nu_1 = (9+\sqrt{6})/36$, $\nu_2 = (9-\sqrt{6})/36$, $\rho_1 = (4-\sqrt{6})/10$, $\rho_2 = (4+\sqrt{6})/10$, $\tau_{21} = (9+\sqrt{6})/50$. These parameters are not unique solution (1.5.1) ~ (1.5.4). The solution of them is represented with one parameter ρ by the following:

$$\rho_1 = \rho \qquad (\rho \neq \tfrac{1}{3}),$$

$$\rho_2 = (2\rho-1)/2(3\rho-1),$$

$$\nu_1 = 1/6(6\rho^2+1),$$

$$\nu_2 = (9\rho^2+1)/3(6\rho^2+1),$$

$$\tau_{21} = (6\rho^2+1)/8(9\rho^2+1)$$

§1 6 Attainable Order of (1,3)-Stage Formula.

The determining equation for the explicit (1,3)-stage formula are given as follows:

(E-0) $\nu_1 + \nu_2 + \nu_3 = \frac{1}{2}$

(E-1) $\nu_1\rho_1 + \nu_2\rho_2 + \nu_3\rho_3 = \frac{1}{6}$

(E-21) $\nu_1\rho_1^2 + \nu_2\rho_2^2 + \nu_3\rho_3^2 = \frac{1}{12}$

(E-22) $\nu_2\tau_{21} + \nu_3(\tau_{31}+\tau_{32}) = \frac{1}{24}$

(E-31) $\nu_1\rho_1^3 + \nu_2\rho_2^3 + \nu_3\rho_3^3 = \frac{1}{20}$

(E-32) $\nu_2\rho_2\tau_{21} + \nu_3\rho_3(\tau_{31}+\tau_{32}) = \frac{1}{40}$

(E-33) $\nu_2\rho_1\tau_{21} + \nu_3(\rho_1\tau_{31}+\rho_2\tau_{32}) = \frac{1}{120}$

(E-41) $\nu_1\rho_1^4 + \nu_2\rho_2^4 + \nu_3\rho_3^4 = \frac{1}{30}$

(E-42) $\nu_2\rho_2^2\tau_{21} + \nu_3\rho_3^2(\tau_{31}+\tau_{32}) = \frac{1}{60}$

(E-43) $\nu_2\rho_2\rho_1\tau_{21} + \nu_3\rho_3(\rho_1\tau_{31} + \rho_2\tau_{32}) = \frac{1}{180}$

(E-44) $\nu_2\rho_1^2\tau_{21} + \nu_3(\rho_1^2\tau_{31} + \rho_2^2\tau_{32}) = \frac{1}{360}$

(E-45) $$\nu_2\tau_{21}^2 + \nu_3(\tau_{31}+\tau_{32})^2 = \frac{1}{120}$$

(E-46) $$\nu_3\tau_{21}\tau_{32} = \frac{1}{720}$$

It is remarkable that none of the factors on the left of (E-46) can vanish.

Assume that two of ρ_1, ρ_2, ρ_3 are equal, say $\rho_I=\rho_J$. Then, from (E-0), (E-1), (E-21), (E-31) and (E-41), we see that

$$\begin{bmatrix} 1 & 1 & \frac{1}{2} \\ \rho_I & \rho_K & \frac{1}{6} \\ \rho_I^2 & \rho_K^2 & \frac{1}{12} \end{bmatrix} \begin{bmatrix} \nu_I+\nu_J \\ \nu_K \\ -1 \end{bmatrix} = 0 ,$$

$$\begin{bmatrix} 1 & 1 & \frac{1}{6} \\ \rho_I & \rho_K & \frac{1}{12} \\ \rho_I^2 & \rho_K^2 & \frac{1}{20} \end{bmatrix} \begin{bmatrix} \rho_I(\nu_I+\nu_J) \\ \rho_K\nu_K \\ -1 \end{bmatrix} = 0 ,$$

$$\begin{bmatrix} 1 & 1 & \frac{1}{12} \\ \rho_I & \rho_K & \frac{1}{20} \\ \rho_I^2 & \rho_K^2 & \frac{1}{30} \end{bmatrix} \begin{bmatrix} \rho_I^2(\nu_I+\nu_J) \\ \rho_K^2\nu_K \\ -1 \end{bmatrix} = 0$$

The condition that the above three equations have non-trivial solutions, implies the equations with respect to ρ_I, ρ_K as follows:

$$(\rho_K-\rho_I)\{\frac{1}{2}\rho_I\rho_K-\frac{1}{6}(\rho_I+\rho_K)+\frac{1}{12}\}=0,$$

$$(\rho_K-\rho_I)\{\frac{1}{6}\rho_I\rho_K-\frac{1}{12}(\rho_I+\rho_K)+\frac{1}{20}\}=0$$

and

$$(\rho_K-\rho_I)\{\frac{1}{12}\rho_I\rho_K-\frac{1}{20}(\rho_I+\rho_K)+\frac{1}{30}\}=0$$

If $\rho_I\neq\rho_K$, ρ_I and ρ_K must satisfy the equations

$$\frac{1}{2}\rho_I\rho_K-\frac{1}{6}(\rho_I+\rho_K)+\frac{1}{12}=\frac{1}{6}\rho_I\rho_K-\frac{1}{12}(\rho_I+\rho_K)+\frac{1}{20}=\frac{1}{12}\rho_I\rho_K-\frac{1}{20}(\rho_I+\rho_K)+\frac{1}{30}=0,$$

which is impossible The case of $\rho_1=\rho_2=\rho_3$ leads to a contradiction because of

$$\nu_1+\nu_2+\nu_3=\frac{1}{2},$$

$$\rho_1(\nu_1+\nu_2+\nu_3)=\frac{1}{6},$$

$$\rho_1^2(\nu_1+\nu_2+\nu_3)=\frac{1}{12},$$

induced by (E-0), (E-1), (E-21), respectively

Hence no two of ρ_1, ρ_2, ρ_3 are equal. It is convenient to define

$$A_i = \sum_{j=1}^{i-1} \tau_{ij} - \frac{1}{2}\rho_i^2 \qquad (i=1,2,3)$$

Since we consider the explicit formula, $A_1=-\frac{1}{2}\rho_1^2$ holds. Then, we have simultaneous linear equations

$$\begin{bmatrix} 1 & 1 & 1 \\ \rho_1 & \rho_2 & \rho_3 \\ \rho_1^2 & \rho_2^2 & \rho_3^2 \end{bmatrix} \begin{bmatrix} \nu_1 A_1 \\ \nu_2 A_2 \\ \nu_3 A_3 \end{bmatrix} = 0$$

by (E-21), (E-22), (E-31), (E-32), (E-41) and (E-42) Since no two of ρ_1, ρ_2, ρ_3 are equal, all of $\nu_1 A_1$, $\nu_2 A_2$, $\nu_3 A_3$ vanish. By virtue of the above mentioned remark, we distinguish the following four cases

Case 1. $A_1 = A_2 = A_3 = 0$

The equations $A_1=0$ and $A_2=0$ imply $\rho_1=0$ and $\tau_{21}=\frac{1}{2}\rho_2^2$. Then, (E-43) and (E-44) bring the equations $\nu_3\rho_2\rho_3\tau_{32}=\frac{1}{180}$ and $\nu_3\rho_2^2\tau_{32}=\frac{1}{360}$, which give the identity $\rho_3 = 2\rho_2$

Thus (E-1), (E-21) and (E-31) imply the equation

$$\begin{bmatrix} \rho_2 & 2\rho_2 & \frac{1}{6} \\ \rho_2^2 & 4\rho_2^2 & \frac{1}{12} \\ \rho_3^3 & 8\rho_3^3 & \frac{1}{20} \end{bmatrix} \begin{bmatrix} \nu_2 \\ \nu_3 \\ -1 \end{bmatrix} = 0,$$

which yields a quadratic equation of ρ_2

$$20\rho_2^2 - 15\rho_2 + 3 = 0$$

because of $\rho_2 \neq 0$. But the above quadratic equation has no real roots

Case 2. $\nu_1=0$ and $A_2 = A_3 = 0$.

In such case, we have the equations

$$\tau_{21} = \frac{1}{2}\rho_2^2$$

and

$$\tau_{31} + \tau_{32} = \frac{1}{2}\rho_3^2 .$$

Substitution of $\tau_{21}=\frac{1}{2}\rho_2^2$ and $\tau_{31}=\frac{1}{2}\rho_3^2-\tau_{32}$ into (E-44) implies

$$\rho_1^2 + 24\nu_3\tau_{32}(\rho_2^2 - \rho_1^2) = \frac{1}{15}$$

Employing the equation

$$(*)\quad \nu_3\rho_2^2\tau_{32} = \frac{1}{360}$$

induced by (E-46), we obtain

$$\rho_1(1 - 24\nu_3\tau_{32}) = 0$$

Hence, the equation $\rho_1=0$ or $\nu_3\tau_{32}=\frac{1}{24}$ holds. The case of $\rho_1=0$ is equivalent to Case 1. The equation $\nu_3\tau_{32}=\frac{1}{24}$ yields

$$\rho_1 + 24\nu_3\tau_{32}(\rho_2 - \rho_1) = \rho_2 = \frac{1}{5}$$

by (E-33) The equation (*), however, implies $\rho_2^2=\frac{1}{15}$, which leads to a contradiction

Case 3. $\nu_2 = 0$ and $A_1 = A_3 = 0$

$A_1=0$ implies $\rho_1=0$. Then, (E-1) and (E-21) bring the equations

$$\nu_3\rho_3 = \frac{1}{6}$$

and

$$\nu_3\rho_3^2 = \frac{1}{12}\,.$$

Hence we see $\rho_3=\frac{1}{2}$ and $\nu_3=\frac{1}{3}$. It contradicts the equation $\nu_3\rho_3^3=\frac{1}{20}$ induced by (E-31)

Case 4. $\nu_1=0$, $\nu_2=0$ and $A_3=0$.

The equations (E-0) and (E-1) yield $\nu_3=\frac{1}{2}$ and $\rho_3=\frac{1}{3}$. Again, it contradicts the equation $\nu_3\rho_3^3=\frac{1}{20}$ induced by (E-31).

Thus, we can conclude that the determining equations (E-0) ∿ (E-46) have no solutions. The proof of the following theorem is now accomplished.

Theorem 7 The explicit (1,3)-stage formula can not attain order 6 Its attainable order is 5.

Note. Shintani gives (1,3)-stage formula with parameters

$$\nu_1 = \frac{1}{12},\ \nu_2 = (5+\sqrt{5})/24,\ \nu_3 = (5-\sqrt{5})/24,\ \rho_1 = 0,\ \rho_2 = (5-\sqrt{5})/10.$$

$\tau_{21} = (3-\sqrt{5})/20$, $\rho_3 = (5+\sqrt{5})/10$, $\tau_{31} = 0$ and $\tau_{32} = (3+\sqrt{5})/20$

These parameters are also not unique solution of (E-0)$\sim$(E-33).

§1.7 Attainable Order of (1,4)-Stage Formula.

The determining equation for the explicit (1,4)-stage formula are given by the following:

(E-0) $\nu_1+\nu_2+\nu_3+\nu_4 = \frac{1}{2}$

(E-1) $\nu_1\rho_1+\nu_2\rho_2+\nu_3\rho_3+\nu_4\rho_4 = \frac{1}{6}$

(E-21) $\nu_1\rho_1^2+\nu_2\rho_2^2+\nu_3\rho_3^2+\nu_4\rho_4^2 = \frac{1}{12}$

(E-22) $\nu_2\tau_{21}+\nu_3(\tau_{31}+\tau_{32})+\nu_4(\tau_{41}+\tau_{42}+\tau_{43}) = \frac{1}{24}$

(E-31) $\nu_1\rho_1^3+\nu_2\rho_2^3+\nu_3\rho_3^3+\nu_4\rho_4^3 = \frac{1}{20}$

(E-32) $\nu_2\rho_2\tau_{21}+\nu_3\rho_3(\tau_{31}+\tau_{32})+\nu_4\rho_4(\tau_{41}+\tau_{42}+\tau_{43}) = \frac{1}{40}$

(E-33) $\nu_2\rho_1\tau_{21}+\nu_3(\rho_1\tau_{31}+\rho_2\tau_{32})+\nu_4(\rho_1\tau_{41}+\rho_2\tau_{42}+\rho_3\tau_{43}) = \frac{1}{120}$

(E-41) $\nu_1\rho_1^4+\nu_2\rho_2^4+\nu_3\rho_3^4+\nu_4\rho_4^4 = \frac{1}{30}$

(E-42) $\nu_2\rho_2^2\tau_{21}+\nu_3\rho_3^2(\tau_{31}+\tau_{32})+\nu_4\rho_4^2(\tau_{41}+\tau_{42}+\tau_{43}) = \frac{1}{60}$

(E-43) $\nu_2\rho_2\rho_1\tau_{21}+\nu_3\rho_3(\rho_1\tau_{31}+\rho_2\tau_{32})+\nu_4\rho_4(\rho_1\tau_{41}+\rho_2\tau_{42}+\rho_3\tau_{43}) = \frac{1}{180}$

(E-44) $\nu_2\rho_1^2\tau_{21}+\nu_3(\rho_1^2\tau_{31}+\rho_2^2\tau_{32})+\nu_4(\rho_1^2\tau_{41}+\rho_2^2\tau_{42}+\rho_3^2\tau_{43}) = \frac{1}{360}$

(E-45) $\nu_3\tau_{21}\tau_{32}+\nu_4(\tau_{21}\tau_{42}+\tau_{31}\tau_{43}+\tau_{32}\tau_{43}) = \frac{1}{720}$

(E-46) $\nu_2\tau_{21}^2+\nu_3(\tau_{31}+\tau_{32})^2+\nu_4(\tau_{41}+\tau_{42}+\tau_{43})^2 = \frac{1}{120}$

(E-51) $\nu_1\rho_1^5+\nu_2\rho_2^5+\nu_3\rho_3^5+\nu_4\rho_4^5 = \frac{1}{42}$

(E-52) $\nu_2\rho_2^3\tau_{21}+\nu_3\rho_3^3(\tau_{31}+\tau_{32})+\nu_4\rho_4^3(\tau_{41}+\tau_{42}+\tau_{43}) = \frac{1}{84}$

(E-53) $\nu_2\rho_2^2\rho_1\tau_{21}+\nu_3\rho_3^2(\rho_1\tau_{31}+\rho_2\tau_{32})+\nu_4\rho_4^2(\rho_1\tau_{41}+\rho_2\tau_{42}+\rho_3\tau_{43})=\frac{1}{252}$

(E-54) $\nu_2\rho_2\rho_1^2\tau_{21}+\nu_3\rho_3(\rho_1^2\tau_{31}+\rho_2^2\tau_{32})+\nu_4\rho_4(\rho_1^2\tau_{41}+\rho_2^2\tau_{42}+\rho_3^2\tau_{43})=\frac{1}{504}$

(E-55) $\nu_2\rho_1^3\tau_{21}+\nu_3(\rho_1^3\tau_{31}+\rho_2^3\tau_{32})+\nu_4(\rho_1^3\tau_{41}+\rho_2^3\tau_{42}+\rho_3^3\tau_{43}) = \frac{1}{840}$

(E-56) $\nu_3(\rho_2+\rho_3)\tau_{21}\tau_{32}+\nu_4(\rho_2+\rho_4)\tau_{21}\tau_{42}+\nu_4(\rho_3+\rho_4)(\tau_{31}\tau_{43}+\tau_{32}\tau_{43})=\frac{1}{630}$

(E-57) $\nu_3\rho_1\tau_{21}\tau_{32}+\nu_4\rho_1(\tau_{21}\tau_{42}+\tau_{31}\tau_{43})+\nu_4\rho_2\tau_{32}\tau_{43}= \frac{1}{5040}$

(E-58) $\nu_2\rho_1\tau_{21}^2+\nu_3(\rho_1\tau_{31}^2+\rho_1\tau_{31}\tau_{32}+\rho_2\tau_{31}\tau_{32}+\rho_2\tau_{32}^2)+\nu_4(\rho_1\tau_{41}^2+\rho_2\tau_{42}^2+\rho_3\tau_{43}^2)$

$+\nu_4\rho_1(\tau_{41}\tau_{42}+\tau_{41}\tau_{43})+\nu_4\rho_2(\tau_{41}\tau_{42}+\tau_{42}\tau_{43})+\nu_4\rho_3(\tau_{31}\tau_{43}+\tau_{42}\tau_{43})$

$= \frac{1}{504}$

(E-59) $\nu_2\rho_2\tau_{21}^2+\nu_3\rho_3(\tau_{31}+\tau_{32})^2+\nu_4\rho_4(\tau_{41}+\tau_{42}+\tau_{43})^2 = \frac{1}{168}$

The question is whether any parameters ν_i, ρ_i and τ_{ij} exist to satisfy these 22 equations simultaneously It is helpful for investigation to introduce the following notations:

$$T_{i0} = \sum_{j=1}^{i-1} \tau_{ij}, \quad T_{i1} = \sum_{j=1}^{i-1} \rho_j \tau_{ij} \qquad (i=1,2,3,4)$$

(T_{10} and T_{11} mean zero.)

$$A_i = T_{i0} - \frac{1}{2}\rho_i^2, \quad B_i = T_{i1} - \frac{1}{6}\rho_i^3 \quad (i=1,2,3,4).$$

Then, from (E-21), (E-22), (E-31), (E-32), (E-33), (E-41), (E-42), (E-43), (E-51), (E-52) and (E-53), we easily see that

$$(1.7.1) \quad \sum_i \nu_i A_i = \sum_i \nu_i \rho_i A_i = \sum_i \nu_i \rho_i^2 A_i = \sum_i \nu_i \rho_i^3 A_i = 0$$

and

$$(1.7\ 2) \quad \sum_i \nu_i B_i = \sum_i \nu_i \rho_i B_i = \sum_i \nu_i \rho_i^2 B_i = 0.$$

The equations (1) means

$$\begin{pmatrix} 1 & 1 & 1 & 1 \\ \rho_1 & \rho_2 & \rho_3 & \rho_4 \\ \rho_1^2 & \rho_2^2 & \rho_3^2 & \rho_4^2 \\ \rho_1^3 & \rho_2^3 & \rho_3^3 & \rho_4^3 \end{pmatrix} \begin{pmatrix} \nu_1 A_1 \\ \nu_2 A_2 \\ \nu_3 A_3 \\ \nu_4 A_4 \end{pmatrix} = 0$$

We now distinguish two cases according as two of ρ_1, ρ_2, ρ_3, ρ_4 are equal or otherwise

Case 1. Two of ρ_1, ρ_2, ρ_3, ρ_4 are equal

Assume that two of them are equal, say $\rho_I = \rho_J$

Equations (E-0), (E-1), (E-21), (E-31), (E-41) and (E-51) give three simultaneous linear equations as follows:

$$\begin{pmatrix} 1 & 1 & 1 & \frac{1}{2} \\ \rho_I & \rho_K & \rho_L & \frac{1}{6} \\ \rho_I^2 & \rho_K^2 & \rho_L^2 & \frac{1}{12} \\ \rho_I^3 & \rho_K^3 & \rho_L^3 & \frac{1}{20} \end{pmatrix} \begin{pmatrix} \nu_I+\nu_J \\ \nu_K \\ \nu_L \\ -1 \end{pmatrix} = 0,$$

$$\begin{pmatrix} 1 & 1 & 1 & \frac{1}{6} \\ \rho_I & \rho_K & \rho_L & \frac{1}{12} \\ \rho_I^2 & \rho_K^2 & \rho_L^2 & \frac{1}{20} \\ \rho_I^3 & \rho_K^3 & \rho_L^3 & \frac{1}{30} \end{pmatrix} \begin{pmatrix} \rho_I(\nu_I+\nu_K) \\ \rho_K\nu_K \\ \rho_L\nu_K \\ -1 \end{pmatrix} = 0,$$

$$\begin{pmatrix} 1 & 1 & 1 & \frac{1}{12} \\ \rho_I & \rho_K & \rho_L & \frac{1}{20} \\ \rho_I^2 & \rho_K^2 & \rho_L^2 & \frac{1}{30} \\ \rho_I^3 & \rho_K^3 & \rho_L^3 & \frac{1}{42} \end{pmatrix} \begin{pmatrix} \rho_I^2(\nu_I+\nu_J) \\ \rho_K^2\nu_K \\ \rho_L^2\nu_L \\ -1 \end{pmatrix} = 0$$

The condition that these equations have non-trivial solutions, implies the determinants of matrices to be vanishing. Hence, we see that the equations

$$\frac{1}{60}(\rho_I-\rho_K)(\rho_K-\rho_L)(\rho_L-\rho_I)\{-30\rho_I\rho_K\rho_L+10(\rho_I\rho_K+\rho_K\rho_L+\rho_L\rho_I)$$

$$-5(\rho_I+\rho_K+\rho_L)+3\} = 0,$$

$$\frac{1}{60}(\rho_I-\rho_K)(\rho_K-\rho_L)(\rho_L-\rho_I)\{-10\rho_I\rho_K\rho_L+5(\rho_I\rho_K+\rho_K\rho_L+\rho_L\rho_I)$$

$$-3(\rho_I+\rho_K+\rho_L)+2\} = 0$$

and

$$\frac{1}{420}(\rho_I-\rho_K)(\rho_K-\rho_L)(\rho_L-\rho_I)\{-35\rho_I\rho_K\rho_L+21(\rho_I\rho_K+\rho_K\rho_L+\rho_L\rho_I)$$

$$-14(\rho_I+\rho_K+\rho_L)+10\} = 0$$

hold. We can distinguish three cases.

(i) At least three of ρ_i are equal.

(ii) $\rho_I = \rho_J$ and $\rho_K = \rho_L$

(iii) ρ_I, ρ_k, ρ_L are distinct, and the above equations hold.

But, the case (i) can not hold by the similar reason mentioned at the first part of §1.6. In the case (ii), (E-0), (E-1), (E-21), (E-31) and (E-41) imply the equations

$$\begin{pmatrix} 1 & 1 & \frac{1}{2} \\ \rho_I & \rho_K & \frac{1}{6} \\ \rho_I^2 & \rho_K^2 & \frac{1}{12} \end{pmatrix} \begin{pmatrix} \nu_I+\nu_J \\ \nu_K+\nu_L \\ -1 \end{pmatrix} = 0,$$

$$\begin{pmatrix} 1 & 1 & \frac{1}{6} \\ \rho_I & \rho_K & \frac{1}{12} \\ \rho_I^2 & \rho_K^2 & \frac{1}{20} \end{pmatrix} \begin{pmatrix} \rho_I(\nu_I+\nu_J) \\ \rho_K(\nu_K+\nu_L) \\ -1 \end{pmatrix} = 0,$$

$$\begin{pmatrix} 1 & 1 & \frac{1}{12} \\ \rho_I & \rho_K & \frac{1}{20} \\ \rho_I^2 & \rho_K^2 & \frac{1}{30} \end{pmatrix} \begin{pmatrix} \rho_I^2(\nu_I+\nu_J) \\ \rho_K^2(\nu_K+\nu_L) \\ -1 \end{pmatrix} = 0$$

Thus, by the same reason as for case (i), these equations lead to a contradiction.

In the case (iii), we easily see the equations

$$\rho_I + \rho_K + \rho_L = \frac{9}{7},$$

$$\rho_I\rho_K + \rho_K\rho_L + \rho_L\rho_I = \frac{3}{7}$$

and

$$\rho_I\rho_K\rho_L = \frac{1}{35},$$

which imply that ρ_I, ρ_K, ρ_L are distinct roots of the cubic equation

$$(1.7\ 3) \qquad x^3 - \frac{9}{7}x^2 + \frac{3}{7}x - \frac{1}{35} = 0$$

The cubic equaton is irreducible and has three distinct real roots given as follows:

Let θ be an angle such that

$$(1.7\ 4) \qquad \cos 3\theta = \frac{1}{5\sqrt{2}} \qquad (0 < 3\theta \leq \frac{\pi}{2}).$$

Then, the roots are

$$(1.7\ 5) \qquad \begin{cases} R_0 = \frac{1}{7}(3+2\sqrt{2}\cos\theta), \\ R_1 = \frac{1}{7}(3-\sqrt{2}\cos\theta + \sqrt{6}\sin\theta), \\ R_{-1} = \frac{1}{7}(3-\sqrt{2}\cos\theta - \sqrt{6}\sin\theta) \end{cases}$$

Some algebraic properties on the equation (3) are the followings:

Lemma 1 7.1. The roots R_0, R_1, R_{-1} are equal to none of 0, $\frac{1}{7}$, $\frac{1}{3}$.

Proof Substitution of 0, $\frac{1}{7}$ and $\frac{1}{3}$ into the cubic polynomial of (3) gives $-\frac{1}{35}$, $\frac{16}{1715}$ and $\frac{8}{945}$, respectively □

Lemma 1 7.2 The equation (3) has no common roots with the cubic equation

$$(1\ 7\ 6) \qquad x^3 - \frac{3}{8}x^2 - \frac{3}{16}x + \frac{3}{64} = 0$$

Proof Put

$$f_1(x) = x^3 - \frac{9}{7}x^2 + \frac{3}{7}x - \frac{1}{35}$$

and

$$f_2(x) = x^3 - \frac{3}{8}x^2 - \frac{3}{16}x + \frac{3}{64}.$$

The Sylvester's determinant $D(f_1, f_2)$ is equal to $-3437/32768000$. □

Lemma 1.7.3. The equation (3) has no roots, one of which is the triple of another.

Proof Assume that one of roots is equal to the triple of another, then the root satisfy another cubic equation

$$27x^3 - \frac{81}{7}x^2 + \frac{9}{7}x - \frac{1}{35} = 0.$$

That is,

$$x^3 - \frac{3}{7}x^2 + \frac{1}{21}x - \frac{1}{945} = 0$$

Put

$$f_1(x) = x^3 - \frac{9}{7}x^2 + \frac{3}{7}x - \frac{1}{35}$$

and

$$f_2(x) = x^3 - \frac{3}{7}x^2 + \frac{1}{21}x - \frac{1}{945}$$

The Sylvester's determinant $D(f_1, f_2)$ is equal to $80384/41351522625$ □

Case 1 1. $\rho_1 = \rho_2$.

From (E-45) and (E-57), the assumption gives $\rho_1 = \rho_2 = \frac{1}{7}$. Due to Lemma 1.7.1, we lead to a contradiction.

Case 1.2. $\rho_1 \neq \rho_3$

We may assume that ρ_1, ρ_2, ρ_4 are distinct. From (E-0), (E-1) and (E-21), we have the equation

$$(1.7\ 9) \qquad \begin{pmatrix} 1 & 1 & 1 \\ \rho_1 & \rho_2 & \rho_4 \\ \rho_1^2 & \rho_2^2 & \rho_4^2 \end{pmatrix} \begin{pmatrix} \nu_1+\nu_3 \\ \nu_2 \\ \nu_4 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{6} \\ \frac{1}{12} \end{pmatrix}$$

The solution of (9) is given by

$$\begin{pmatrix} \nu_1+\nu_3 \\ \nu_2 \\ \nu_4 \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 \\ \rho_1 & \rho_2 & \rho_4 \\ \rho_1^2 & \rho_2^2 & \rho_4^2 \end{pmatrix}^{-1} \begin{pmatrix} \frac{1}{2} \\ \frac{1}{6} \\ \frac{1}{12} \end{pmatrix}$$

$$= \begin{bmatrix} \dfrac{-6\rho_2\rho_4+2(\rho_2+\rho_4)-1}{12(\rho_1-\rho_2)(\rho_4-\rho_1)} \\ \\ \dfrac{-6\rho_4\rho_1+2(\rho_4+\rho_1)-1}{12(\rho_1-\rho_2)(\rho_2-\rho_4)} \\ \\ \dfrac{-6\rho_1\rho_2+2(\rho_1+\rho_2)-1}{12(\rho_2-\rho_4)(\rho_4-\rho_1)} \end{bmatrix}$$

Note that $\nu_1+\nu_3$, ν_2, ν_4 can not vanish. The reason is as follows: For example, assume that $-6\rho_2\rho_4+2(\rho_2+\rho_4)-1 = 0$ Then,

$$4 = \frac{2\rho_2 - 1}{6\rho_2 - 2}$$

Holds Substituting this into the cubic equation

$$\rho_4^3 - \frac{9}{7}\rho_4^2 + \frac{3}{7}\rho_4 - \frac{1}{35} = 0,$$

we see that

$$\frac{64\rho_2^3 - 24\rho_2^2 - 12\rho_2 + 3}{35(6\rho_2-2)^3} = 0$$

But, by Lemma 1.7.2, there is no common roots for the cubic equations

$$\rho_2^3 - \frac{9}{7}\rho_2^2 + \frac{3}{7}\rho_2 - \frac{1}{35} = 0$$

and

$$\rho_2^3 - \frac{3}{8}\rho_2^2 - \frac{3}{16}\rho_2 + \frac{3}{64} = 0$$

Then, from the equations (1) and (2) we have

$$\nu_1 A_1 + \nu_3 A_3 = \nu_2 A_2 = \nu_4 A_4 = 0$$

and

$$\nu_1 B_1 + \nu_3 B_3 = \nu_2 B_2 = \nu_4 B_4 = 0.$$

Since $\nu_2 \neq 0$, $A_2=B_2=0$ holds This means the equations $\tau_{21} = \frac{1}{2}\rho_2^2$ and $\rho_1\tau_{21} = \frac{1}{6}\rho_2^3$, which imply $3\rho_1 = \rho_2$ Hence, we lead to a contradiction by virture of Lemma 1.7 3

Case 1.3. $\rho_1 = \rho_4$

This is equivalent to Case 1.2

Case 1.4 $\rho_2 = \rho_3$

We can assume that ρ_1, ρ_2, ρ_4 are distinct. From (E-0), (E-1), (E-21), we have the solution

$$\nu_1 = \frac{-6\rho_2\rho_4 + 2(\rho_2+\rho_4)-1}{12(\rho_1-\rho_2)(\rho_4-\rho_1)}$$

$$\nu_2+\nu_3 = \frac{-6\rho_4\rho_1 + 2(\rho_4+\rho_1)-1}{12(\rho_1-\rho_2)(\rho_2-\rho_4)},$$

$$\nu_4 = \frac{-6\rho_1\rho_2 + 2(\rho_1+\rho_2)-1}{12(\rho_2-\rho_4)(\rho_4-\rho_1)}$$

Note that each numerator on the right can not vanish by the same reason as in Case 1.2 Then, (1) implies $\nu_1 A_1 = \nu_2 A_2 + \nu_3 A_3 = \nu_4 A_4 = 0$ Since $\nu_1 \neq 0$, we see $A_1 = 0$, which means $\rho_1 = 0$. Thus, we lead to a contradiction.

Case 1.5. $\rho_2 = \rho_4$

and

Case 1.6. $\rho_3 \quad \rho_4$

Both of them are equivalent to Case 1.4.

Case 2. No two of ρ_1, ρ_2, ρ_3, ρ_4 are equal.

The equation (1) implies $\nu_1 A_1 = \nu_2 A_2 = \nu_3 A_3 = \nu_4 A_4 = 0$ Thus, we distinguish cases according as ν_i or A_i vanishes. We have, however, the following results.

Lemma 1.7.4 The case of $\nu_J = \nu_K - \nu_L = 0$ can not occur

Proof In this case, $\nu_I = \frac{1}{2}$ by (E-0). Then, (E-1) implies $\rho_I = \frac{1}{3}$ But, they do not satisfy (E-21). □

Lemma 1 7 5 The case for $\nu_K = \nu_L = 0$ leads to a contradiction.

Proof The equation $\nu_K - \nu_L = 0$ yields a linear system

$$\nu_I + \nu_J = \frac{1}{2},$$

$$\rho_I \nu_I + \rho_J \nu_J = \frac{1}{6}$$

by (E-0), (E-1) Since $\rho_I \neq \rho_J$, this system has the solution

$$\nu_I = \frac{1 - 3\rho_J}{6(\rho_I - \rho_J)}, \qquad \nu_J = \frac{1 - 3\rho_I}{6(\rho_J - \rho_I)}$$

Substitution of this into (E-21) and (E-31) implies

$$\frac{1}{6}(\rho_I + \rho_J) - \frac{1}{2}\rho_I\rho_J = \frac{1}{12},$$

$$\frac{1}{6}(\rho_I^2 + \rho_I\rho_J + \rho_J^2) - \frac{1}{2}\rho_I\rho_J(\rho_I + \rho_J) = \frac{1}{20}.$$

Put $X = \rho_I + \rho_J$, $Y = \rho_I\rho_J$, we have

$$2X - 6Y = 1,$$

$$10(X^2 - Y) - 30XY = 3.$$

Thus, we easily see that $X = \frac{4}{5}$, $Y = \frac{1}{10}$. That is, ρ_I and ρ_J are equal to the roots of the quadratic equation

$$x^2 - \frac{4}{5}x + \frac{1}{10} = 0, \tag{1.7.10}$$

which has real distinct roots On the other hand, we see that

$$\text{the left on (E-41)} = \nu_I\rho_I^4 + \nu_J\rho_J^4$$

$$= \frac{1}{6}(\rho_I + \rho_J)(\rho_I^2 + \rho_J^2) - \frac{1}{2}\rho_I\rho_J(\rho_I^2 + \rho_I\rho_J + \rho_J^2)$$

$$= \frac{19}{600}$$

which is a contradiction. □

Due to the above Lemmas, we distinguish five cases.

Case 2.1. $\nu_1 = 0$ and $A_2 = A_3 = A_4 = 0$ By a similar consideration as in Case 1, we see that ρ_2, ρ_3, ρ_4 satisfy

$$\rho_2 + \rho_3 + \rho_4 = \frac{9}{7},$$

$$\rho_2\rho_3 + \rho_3\rho_4 + \rho_4\rho_2 \quad \frac{3}{7},$$

$$\rho_2\rho_3\rho_4 = \frac{1}{35}$$

Hence, they are equal to the distinct roots of the cubic equation (3) Note that, contrary to Case 1, ρ_1 is equal to none of them.

On the other hand, the equation (2) yields $\nu_2 B_2 = \nu_3 B_3 = \nu_4 B_4 = 0$ Taking Lemma 1.7 5 into account, we are sufficient to consider the case $B_2 = B_3 = B_4 = 0$.

$A_2 = B_2 = 0$ implies the equations $\tau_{21} = \frac{1}{2}\rho_2^2$ and $\rho_1\tau_{21} = \frac{1}{6}\rho_2^3$, which give $\rho_1 = \frac{1}{3}\rho_2$ $A_3 = B_3 = 0$ implies a linear system

$$\tau_{31} + \tau_{32} = \frac{1}{2}\rho_3^2,$$

$$\rho_1\tau_{31} + \rho_2\tau_{32} = \frac{1}{6}\rho_3^3,$$

which has the solution

$$(1.7\ 11) \qquad \tau_{31} = \frac{\rho_3^2(3\rho_2-\rho_3)}{4\rho_2}, \qquad \tau_{32} = \frac{\rho_3^2(\rho_3-\rho_2)}{4\rho_2}.$$

Since ρ_2, ρ_3, ρ_4 are distinct, (E-0), (E-1), (E-21) give

the solution for ν_2, ν_3, ν_4 as

$$(1.7\ 12)\qquad \begin{cases} \nu_2 = \dfrac{-6\rho_3\rho_4+2(\rho_3+\rho_4)-1}{12(\rho_2-\rho_3)(\rho_4-\rho_2)}\ , \\ \nu_3 = \dfrac{-6\rho_4\rho_2+2(\rho_4+\rho_2)-1}{12(\rho_2-\rho_3)(\rho_3-\rho_4)}\ , \\ \nu_4 = \dfrac{-6\rho_2\rho_3+2(\rho_2+\rho_3)-1}{12(\rho_3-\rho_4)(\rho_4-\rho_2)} \end{cases}$$

(E-44) gives the equation

$$\begin{aligned} \nu_4(\rho_1^2\tau_{41}+\rho_2^2\tau_{42}+\rho_3^2\tau_{43}) &= \frac{1}{360}-\nu_2\rho_1^2\tau_{21}-\nu_3(\rho_1^2\tau_{31}+\rho_2^2\tau_{32}) \\ &= \frac{1}{360}-\frac{1}{18}\nu_2\rho_2^4-\nu_3\rho_2^2(\frac{1}{9}\tau_{31}+\tau_{32}) \\ &= \frac{1}{360}-\frac{1}{18}\nu_2\rho_2^4-\frac{1}{18}\nu_3\rho_2\rho_3^2(4\rho_3-3\rho_2) \end{aligned}$$

by (9) Hence, we may represent the left on (E-54) as the polynomial of ρ_2 and ρ_3 By (9) and (10),

$$\nu_2\rho_2\rho_1^2\tau_{21}+\nu_3\rho_3(\rho_1^2\tau_{31}+\rho_2^2\tau_{32})+\nu_4\rho_4(\rho_1^2\tau_{41}+\rho_2^2\tau_{42}+\rho_3^2\tau_{43})-\frac{1}{504}$$

$$= \frac{1}{18}\nu_2\rho_2^5+\frac{1}{18}\nu_3\rho_2\rho_3^3(4\rho_3-3\rho_2)+\frac{\rho_4}{360}-\frac{1}{18}\nu_2\rho_2^4\rho_4-\frac{1}{18}\nu_3\rho_2\rho_3^2\rho_4(4\rho_3-3\rho_2)-\frac{1}{504}$$

$$- \frac{1}{37800(\rho_2-\rho_3)}(525\rho_2^2\rho_3^2-360\rho_2^2\rho_3-420\rho_2\rho_3^2-5\rho_2^2+260\rho_2\rho_3+105\rho_3^2-60\rho_3+3)$$

Let us denote the numerator of the above by $\varphi(\rho_2, \rho_3)$

The question is whether $\varphi(\rho_2, \rho_3)$ vanishes for any pair (ρ_2, ρ_3) We have known the values R_0, R_1, R_{-1} which ρ_2 and ρ_3 are possible to be equal to. Calculation shows the following:

$$\varphi(R_0,R_1) = \frac{4}{343}(-420\cos^2\theta-760\sqrt{3}\sin\theta\cdot\cos\theta-630\sqrt{2}\cos\theta+60\sqrt{6}\sin\theta +189+42\sqrt{3}),$$

$$\varphi(R_0,R_{-1}) = \frac{4}{343}(-420\cos^2\theta+760\sqrt{3}\sin\theta\cdot\cos\theta-630\sqrt{2}\cos\theta-60\sqrt{6}\sin\theta +189-42\sqrt{3}),$$

$$\varphi(R_1,R_0) = \frac{4}{343}(1350\cos^2\theta-170\sqrt{3}\cos\theta\cdot\sin\theta+405\sqrt{2}\cos\theta-285\sqrt{6}\sin\theta -696-42\sqrt{3}),$$

$$\varphi(R_1,R_{-1}) = \frac{4}{343}(-930\cos^2\theta+590\sqrt{3}\sin\theta\cdot\cos\theta+225\sqrt{2}\cos\theta-345\sqrt{6}\sin\theta +444+42\sqrt{3}),$$

$$\varphi(R_{-1},R_0) = \frac{4}{343}(1350\cos^2\theta+170\sqrt{3}\sin\theta\cos\theta+405\sqrt{2}\cos\theta+285\sqrt{6}\sin\theta -696+42\sqrt{3}),$$

$$\varphi(R_{-1},R_1) = \frac{4}{343}(-930\cos^2\theta-590\sqrt{3}\sin\theta\cdot\cos\theta+225\sqrt{2}\cos\theta+345\sqrt{6}\sin\theta +444-42\sqrt{3})$$

Computation by interval arithmetic shows the following:

$$\varphi(R_0, R_1) \in [-11.6391, -11.6390],$$

$$\varphi(R_0, R_{-1}) \in [-4.70784, -4\ 70783],$$

$$\varphi(R_1, R_0) \in [3.20479, 3.20480],$$

$$\varphi(R_1, R_{-1}) \in [0\ 821791, 0.821792],$$

$$\varphi(R_{-1}, R_0) \in [12.1750, 12.1751],$$

$$\varphi(R_{-1}, R_1) \in [-0\ 956777, -0.956776]$$

(On the interval arithmetic, see [8] Above calculation is carried out by the program made by K. Ichida on HITAC VOS3 at the Educational Center for Information Processing, Kyoto Univ) None of them vanishes under the condition (4) because every interval given above is away from zero Thus, we have a contradiction.

Case 2 2. $\nu_2 = 0$ and $A_1=A_3=A_4=0$ $A_1 = 0$ implies $\rho_1=0$ Then, ρ_2, ρ_3, ρ_4 can not vanish. From (E-1), (E-21), we have

$$\nu_3 = \frac{1-2\rho_4}{12\rho_3(\rho_3-\rho_4)}, \qquad \nu_4 = \frac{1-2\rho_3}{12\rho_4(\rho_4-\rho_3)}.$$

Substituting these into (E-31), (E-41), we see that

$$\rho_3 + \rho_4 - 2\rho_3\rho_4 = \frac{3}{5},$$

$$(\rho_3+\rho_4)^2 - 2\rho_3\rho_4(\rho_3+\rho_4) - \rho_3\rho_4 = \frac{2}{5}.$$

Put $X = \rho_3+\rho_4$, $Y = \rho_3\rho_4$, then we have $X = 1$, $Y = \frac{1}{5}$. The left on (E-51) is equal to

$$\frac{1}{12}(-2\rho_3^3\rho_4-2\rho_3\rho_4^3-2\rho_3^2\rho_4^2+\rho_3^3+\rho_3^2\rho_4+\rho_3\rho_4^2+\rho_4^3)$$

$$= \frac{1}{12}\{X^3-2(X^2-Y)Y-2(X+Y)Y\} = \frac{1}{100} ,$$

which is a contradiction.

Case 2 3 $\nu_3 = 0$ and $A_1=A_2=A_4=0$. Equivalent to Case 2.2

Case 2.4 $\nu_4 = 0$ and $A_1=A_2=A_3=0$ Equivalent to Case 2.2.

Case 2.5. $A_1=A_2=A_3=A_4=0$. $A_1=0$ implies $\rho_1=0$, which means $B_1=0$. Then, the equations $\sum\nu_iB_i = \sum\nu_i\rho_iB_i = \sum\nu_i\rho_i^2B_i = 0$ yield $\nu_2B_2 = \nu_3B_3 = \nu_4B_4 = 0$ Since ν_2, ν_3, ν_4 are assumed to be non-zero, we have $B_2 = B_3 = B_4 = 0$ $B_2 = \rho_1\tau_{21}-\frac{1}{6}\rho_2^3 = 0$ implies $\rho_2 = 0$ because $\rho_1 = 0$. This contradicts the assumption that no two of ρ_i are equal.

Now, we have accomplished to investigate the whole cases. In conclusion, we have

Theorem 8 The explicit (1,4)-stage formula can not attain order 7 Its attainable order is 6.

Note. Shintani gives (1,4)-stage formula with parameters $v_1 = \frac{1}{20}$, $v_2 = 7(7+\sqrt{21})/360$, $v_3 = 8/45$, $v_4 = 7(7-\sqrt{21})/360$, $\rho_1 = 0$, $\rho_2 = (7-\sqrt{21})/14$, $\tau_{21} = (5-\sqrt{21})/28$, $\rho_3 = \frac{1}{2}$, $\tau_{31} = (3-\sqrt{21})/192$, $\tau_{32} = (21+\sqrt{21})/192$, $\rho_4 = (7+\sqrt{21})/14$, $\tau_{41} = (21+5\sqrt{21})/294$, $\tau_{42} = (\sqrt{21}-3)/84$, $\tau_{43} = (21+\sqrt{21})/147$ These parameters are also not unique solution of (E-0) ~ (E-46).

References

[1] Butcher, J. C., Coefficients for the study of Runge-Kutta integration processes, J Austral Math. Soc., 3 (1963), 185-201.

[2] _____, On Runge-Kutta processes of high order, J. Austral. Math. Soc., 4 (1964), 179-194.

[3] _____, Implicit Runge-Kutta processes, Math. Comput., 18 (1964), 50-64.

[4] _____, On the attainable order of Runge-Kutta methods, Math. Comput., 19 (1965), 408-417

[5] Cash, J R., High order methods for the numerical integration of ordinary differential equations, Numer. Math., 30 (1978), 385-409.

[6] Hearn, A. C., REDUCE 2 User's Manual, second ed., Univ Utah, March 1973.

[7] Kaps, P and Rentrop. P , Generalized Runge-Kutta methods of order four with stepsize control for stiff ordinary differential equations, Numer. Math., 33 (1979), 55-68.

[8] Moore, R. E., Interval Analysis, Prentice-Hall Inc , New Jersey, 1966.

[9] Nørsett, S. P and Walfbrandt, A., Order conditions for Rosenbrook-type method, Numer. Math., 32 (1979), 1-15

[10] Riordan, J , Derivatives of composite functions, Bull. A. M. S., 52 (1946), 664-667

[11] Rosenbrook, H. H., Some general implicit processes for the numerical solution of differential equations. Computer J , 5 (1963), 329-330.

[12] Shintani, H., On one-step methods utilizing the second derivative, Hiroshima Math. J , 1 (1971), 349-372

[13] _____, On explicit one-step methods utilizing the second derivative, Hiroshima Math. J , 2 (1972), 353-368.

[14] Toda, H., On the truncation error of a limiting formula of Runge-Kutta methods, Res. Electrotech. Lab., No.772, 1977

[15] Urabe, M., An implicit one-step method of high order accuracy for the numerical integration of ordinary differential equations, Numer. Math , 15 (1970), 151-164.

Table 1.

$$\kappa_0 = g_0$$

$$\kappa_1 = [D_0 g]_0$$

$$\kappa_2 = [D_0^2 g]_0 + g_0\, g_{y,0}$$

$$\kappa_3 = [D_0^3 g]_0 + [D_0 g]_0\, g_{y,0} + 3g_0\, [D_0 g_y]_0$$

$$\kappa_4 = [D_0^4 g]_0 + [D_0^2 g]_0\, g_{y,0} + 4[D_0 g]_0\, [D_0 g_y]_0 + 6g_0\, [D_0^2 g_y]_0 + g_0\, g_{y,0}^2 + 3g_0^2\, g_{yy,0}$$

$$\kappa_5 = [D_0^5\, g]_0 + [D_0^3 g]_0\, g_{y,0} + 5[D_0^2 g]_0\, [D_0 g_y]_0 + 10[D_0 g]_0\, [D_0^2 g_y]_0 + 10g_0\, [D_0^3 g_y]_0 + [D_0 g]_0\, g_{y,0}^2 + 8g_0 \cdot g_{y,0}\, [D_0 g_y]_0 + 10g_0\, [D_0 g]_0 \cdot g_{yy,0} + 15g_0^2 \cdot [D_0 g_{yy}]_0$$

$$\kappa_6 = [D_0^6 g]_0 + [D_0^4 g]_0\, g_{y,0} + 6[D_0^3 g]_0\, [D_0 g_y]_0 + 15[D_0^2 g]_0\, [D_0^2 g_y]_0 + 20[D_0 g]_0\, [D_0^3 g_y]_0 + 15g_0\, [D_0^4 g_y]_0 + [D_0^2 g]_0\, g_{y,0}^2 + 18g_0\, [D_0 g_y]_0^2 + 10[D_0 g]_0\, g_{y,0}\, [D_0 g_y]_0 + 21g_0\, g_{y,0}\, [D_0^2 g_y]_0 + 10[D_0 g]_0^2\, g_{yy,0} + 15g_0\, [D_0^2 g]_0\, g_{yy,0} + 60g_0\, [D_0 g]_0\, [D_0 g_{yy}]_0 + 45g_0^2 \cdot [D_0^2 g_{yy}]_0$$

$$+ g_0 \cdot g_{y,0}^3 + 18 g_0^2 \cdot g_{y,0} \cdot g_{yy,0} + 15 g_0^3 \cdot g_{yyy,0}$$

$$\kappa_7 = [D_0^7 g]_0 + [D_0^5 g] \cdot g_{y,0} + 7[D_0^4 g]_0 \, [D_0 g_y]_0 + 21[D_0^3 g]_0 \, [D_0^2 g_y]_0$$

$$+ [D_0^3 g]_0 \cdot g_{y,0}^2 + 35[D_0^2 g]_0 \, [D_0^3 g_y]_0 + 12[D_0^2 g]_0 \, g_{y,0} \, [D_0 g_y]_0$$

$$+ 35[D_0 g]_0 \, [D_0^4 g_y]_0 + 28[D_0 g]_0 \, [D_0 g_y]_0^2 + 31[D_0 g]_0 \cdot g_{y,0} \, [D_0^2 g_y]_0$$

$$+ [D_0 g]_0 \, g_{y,0}^3 + 35[D_0 g]_0 \, [D_0^2 g]_0 \cdot g_{yy,0} + 70[D_0 g]_0^2 \, [D_0 g_{yy}]_0$$

$$+ 21 g_0 \, [D_0^5 g_y]_0 + 105 g_0 \, [D_0 g_y]_0 \, [D_0^2 g_y]_0 + 45 g_0 \cdot g_{y,0} \, [D_0^3 g_y]_0$$

$$+ 15 g_0 \, g_{y,0}^2 \, [D_0 g_y]_0 + 21 g_0 \, [D_0^3 g]_0 \, g_{yy,0} + 105 g_0 \, [D_0^2 g]_0 \, [D_0 g_{yy}]_0$$

$$+ 210 g_0 \, [D_0 g]_0 \, [D_0^2 g_{yy}]_0 + 66 g_0 \, [D_0 g]_0 \, g_{y,0} \, g_{yy,0} + 105 g_0^2 \cdot [D_0^3 g_{yy}]_0$$

$$+ 84 g_0^2 \, [D_0 g_y]_0 \cdot g_{yy,0} + 120 g_0^2 \, g_{y,0} \, [D_0 g_{yy}]_0 + 105 g_0^2 \cdot [D_0 g]_0 \cdot g_{yyy,0}$$

$$+ 105 g_0^3 \cdot [D_0 g_{yyy}]_0$$

$$\kappa_8 = [D_0^8 g]_0 + [D_0^6 g]_0 \cdot g_{y,0} + 8[D_0^5 g]_0 \, [D_0 g_y]_0 + 28[D_0^4 g]_0 \, [D_0^2 g_y]_0$$

$$+ [D_0^4 g]_0 g_{y,0}^2 + 56[D_0^3 g]_0 \, [D_0^3 g_y]_0 + 14[D_0^3 g]_0 \, g_{y,0} \, [D_0 g_y]_0$$

$$+ 70[D_0^2 g]_0 \, [D_0^4 g_y]_0 + 40[D_0^2 g]_0 \cdot [D_0 g_y]_0^2 + 43[D_0^2 g]_0 \, g_{y,0} \, [D_0^2 g_y]_0$$

$$+ [D_0^2 g] \, g_{y,0}^3 + 35[D_0^2 g]_0^2 \cdot g_{yy,0} + 56[D_0 g]_0 \, [D_0^5 g_y]_0$$

$$+ 192[D_0 g]_0\ [D_0 g_y]_0\ [D_0^2 g_y]_0 + 76[D_0 g]_0\ g_{y,0} \cdot [D_0^3 g_y]_0$$

$$+ 18[D_0 g]_0 \cdot g_{y,0}^2 \cdot [D_0 g_y]_0 + 56[D_0 g]_0\ [D_0^3 g]_0 \cdot g_{yy,0}$$

$$+ 280[D_0 g]_0\ [D_0^2 g]_0\ [D_0 g_{yy}]_0 + 280[D_0 g]_0^2 \cdot [D_0^2 g_{yy}]_0$$

$$+ 66[D_0 g]_0^2 \cdot g_{y,0}\ g_{yy,0} + 28 g_0\ [D_0^6 g_y]_0 + 168 g_0 \cdot [D_0^2 g_y]_0^2$$

$$+ 248 g_0\ [D_0 g_y]_0 \cdot [D_0^3 g_y]_0 + 85 g_0\ g_{y,0}\ [D_0^4 g_y]_0 + 82 g_0\ g_{y,0} \cdot [D_0 g_y]_0^2$$

$$+ 49 g_0\ g_{y,0}^2\ [D_0^2 g_y]_0 + g_0 \cdot g_{y,0}^4 + 28 g_0\ [D_0^4 g]_0\ g_{yy,0}$$

$$+ 168 g_0\ [D_0^3 g]_0\ [D_0 g_{yy}]_0 + 420 g_0\ [D_0^2 g]_0\ [D_0^2 g_{yy}]_0$$

$$+ 113 g_0\ [D_0^2 g]_0\ g_{y,0}\ g_{yy,0} + 560 g_0\ [D_0 g]_0\ [D_0^3 g_{yy}]_0$$

$$+ 360 g_0\ [D_0 g]_0\ [D_0 g_y]_0\ g_{yy,0} + 508 g_0\ [D_0 g]_0\ g_{y,0}\ [D_0 g_{yy}]_0$$

$$+ 280 g_0\ [D_0 g]_0^2\ g_{yyy,0} + 210 g_0^2 \cdot [D_0^4 g_{yy}]_0$$

$$+ 252 g_0^2\ [D_0^2 g_y]_0 \cdot g_{yy,0} + 624 g_0^2 \cdot [D_0 g_y]_0 \cdot [D_0 g_{yy}]_0$$

$$+ 465 g_0^2 \cdot g_{y,0}\ [D_0^2 g_{yy}]_0 + 81 g_0^2\ g_{y,0}^2\ g_{yy,0} + 210 g_0^2\ [D_0^2 g]_0 \cdot g_{yyy,0}$$

$$+ 840 g_0^2\ [D_0 g]_0\ [D_0 g_{yyy}]_0 + 420 g_0^3 \cdot [D_0^2 g_{yy}]_0 + 84 g_0^3 \cdot g_{yy,0}^2$$

$$+ 225 g_0^3 \cdot g_{y,0}\ g_{yyy,0} + 105 g_0^4\ g_{yyyy,0}$$

Table 2.

$$\kappa_{i0} = g_0$$

$$\kappa_{i1} = \rho_i [D_0 g]_0$$

$$\kappa_{i2} = \rho_i^2 [D_0^2 g]_0 + 2\, T_{i0} \cdot g_0\, g_{y,0}$$

$$\kappa_{i3} = \rho_i^3 [D_0^3 g]_0 + 6\, T_{i1}\, [D_0 g]_0 \cdot g_{y,0} + 6\, \rho_i\, T_{i0} \cdot g_0\, [D_0 g_y]_0$$

$$\kappa_{i4} = \rho_i^4 [D_0^4 g]_0 + 12\, T_{i2} [D_0^2 g]_0\, g_{y,0} + 24 \rho_i T_{i1} [D_0 g]_0\, [D_0 g_y]_0$$

$$+ 12 \rho_i^2 T_{i0}\, g_0\, [D_0^2 g_y]_0 + 24 \left(\sum_j \tau_{ij} T_{j0}\right) g_0\, g_{y,0}^2 + 12\, T_{i0}^2\, g_0^2 \cdot g_{y,0}$$

$$\kappa_{i5} = \rho_i^5\, [D_0^5 g]_0 + 20 T_{i3} \cdot [D_0^3 g]_0\, g_{y,0} + 60 \rho_i T_{i2}\, [D_0^2 g]_0 [D_0 g_y]_0$$

$$+ 60 \rho_i^2 T_{i1} [D_0 g]_0 [D_0^2 g_y]_0 + 120 \left(\sum_j \tau_{ij} T_{j1}\right)\, [D_0 g]_0\, g_{y,0}^2$$

$$+ 20 \rho_i^3 T_{i0} \cdot g_0 \cdot [D_0^3 g_y]_0 + 120 \left\{\sum_j (\rho_i + \rho_j) \tau_{ij} T_{j0}\right\} g_0 \cdot g_{y,0}\, [D_0 g_y]_0$$

$$+ 120 T_{i0} T_{i1}\, g_0\, [D_0 g]_0\, g_{yy,0} + 60 \rho_i T_{i0}^2 \cdot g_0^2 \cdot [D_0 g_{yy}]_0$$

$$\kappa_{i6} = \rho_i^6 [D_0^6 g]_0 + 30 T_{i4} [D_0^4 g]_0\, g_{y,0} + 120 \rho_i T_{i3} [D_0^3 g] \cdot [D_0 g_y]_0$$

$$+ 180 \rho_i^2 T_{i2} [D_0^2 g]_0 [D_0^2 g_y]_0 + 360 \left(\sum_j \tau_{ij} T_{j2}\right) [D_0^2 g]_0\, g_{y,0}^2$$

$$+ 120 \rho_i^3 T_{i1} [D_0 g]_0\, [D_0^3 g_y]_0 + 720 \left\{\sum_j (\rho_i + \rho_j) \tau_{ij} T_{j1}\right\} [D_0 g]_0\, g_{y,0} [D_0 g_y]_0$$

$$+ 360T_{i1}^2[D_0g]_0^2\cdot g_{yy,0} + 30\rho_i^4T_{i0}\, g_0\, [D_0^4g_y]_0$$

$$+ 720(\sum_j\rho_i\rho_j\tau_{ij}T_{j0})\, g_0\, [D_0g_y]_0^2 + 360\{\sum_j(\rho_i^2+\rho_j^2)\tau_{ij}T_{j0}\}g_0\cdot g_{y,0}\cdot[D_0^2g_y]_0$$

$$+ 720(\sum_{jk}\sum\tau_{ij}\tau_{jk}T_{k0})g_0\cdot g_{y,0}^3 + 360T_{i0}T_{i2}\, g_0\, [D_0^2g]_0\cdot g_{yy,0}$$

$$+ 720\rho_iT_{i0}T_{i1}\, g_0\, [D_0g]_0\, [D_0g_{yy}]_0 + 180\rho_i^2T_{i0}^2g_0^2\, [D_0^2g_{yy}]_0$$

$$+ 360\{\sum_j\tau_{ij}(T_{j0}^2+2T_{i0}T_{j0})\}g_0^2\cdot g_{y,0}\, g_{yy,0} + 120T_{i0}^3\cdot g_0^3\cdot g_{yyy,0}$$

$$\kappa_{i7} = \rho_i^7\, [D_0^7g]_0 + 42T_{i5}[D_0^5g]_0\, g_{y,0} + 210\rho_iT_{i4}[D_0^4g]_0\cdot[D_0g_y]_0$$

$$+ 420\rho_i^2T_{i3}[D_0^3g]_0\, [D_0^2g_y]_0 + 840(\sum_j\tau_{ij}T_{j3})[D_0^3g]_0\cdot g_{y,0}^2$$

$$+ 420\rho_i^3T_{i2}[D_0^2g]_0\cdot[D_0^3g_y]_0 + 2520(\sum_j(\rho_i+\rho_j)\tau_{ij}T_{j2})[D_0^2g]_0\cdot g_{y,0}\cdot[D_0g_y]_0$$

$$+ 210\rho_i^4T_{i1}[D_0g]_0\, [D_0^4g_y]_0 + 5040(\sum_j\rho_i\rho_j\tau_{ij}T_{j1})[D_0g]_0\, [D_0g_y]_0^2$$

$$+ 2520(\sum_j(\rho_i^2+\rho_j^2)\tau_{ij}T_{j1})[D_0g]_0\, g_{y,0}\, [D_0^2g_y]_0$$

$$+ 5040(\sum_{jk}\sum\tau_{ij}\tau_{jk}T_{k1})[D_0g]_0\cdot g_{y,0}^3 + 2520T_{i1}T_{i2}[D_0g]_0\, [D_0^2g]_0\cdot g_{yy,0}$$

$$+ 2520\rho_iT_{i1}^2[D_0g]_0^2\, [D_0g_{yy}]_0 + 42\rho_i^5T_{i0}g_0\, [D_0^5g_y]_0$$

$$+ 2520(\sum_j\rho_i\rho_j(\rho_i+\rho_j)\tau_{ij}T_{j0})g_0\, [D_0g_y]_0\, [D_0^2g_y]_0$$

$$+ 840(\sum_j(\rho_i^3+\rho_j^3)\tau_{ij}T_{j0})g_0\cdot g_{y,0}\, [D_0^3g_y]_0$$

$$+ 5040(\sum_{jk}(\rho_i+\rho_j+\rho_k)\tau_{ij}\tau_{jk}T_{k0})g_0\cdot g_{y,0}^2\ [D_0g_y]_0$$

$$+ 840T_{i0}T_{i3}g_0\ [D_0^3g]_0\cdot g_{yy,0} + 2520\rho_iT_{i0}T_{i2}g_0\ [D_0^2g]_0\cdot[D_0g_{yy}]_0$$

$$+ 2520\rho_i^2T_{i0}T_{i1}g_0\ [D_0g]_0\ [D_0^2g_{yy}]_0 + 5040(\sum_j\tau_{ij}(T_{i0}T_{j1}+T_{j0}T_{j1}+T_{j0}T_{i1}))g_0\cdot$$

$$[D_0g]_0\ g_{y,0}\ g_{yy,0} + 420\rho_i^3\ T_{i0}^2g_0^2\cdot[D_0^3g_{yy}]_0$$

$$+ 2520(\sum_j(2\rho_iT_{i0}+\rho_jT_{j0})\tau_{ij}T_{j0})g_0^2\cdot[D_0g_y]_0\cdot g_{yy,0}$$

$$+ 2520(\sum_j(\rho_iT_{j0}+2\rho_jT_{i0})\tau_{ij}T_{j0})g_0^2\cdot g_{y,0}\cdot[D_0g_{yy}]_0$$

$$+ 2520T_{i0}^2T_{i1}g_0^2\ [D_0g]_0\cdot g_{yyy,0} + 840\rho_iT_{i0}^3g_0^3\cdot[D_0g_{yyy}]_0$$

$$\kappa_{i8} = \rho_i^8[D_0^8g]_0 + 56T_{i6}\cdot[D_0^6g]_0\cdot g_{y,0} + 336\rho_iT_{i5}[D_0^5g]_0\ [D_0g_y]_0$$

$$+ 840\rho_i^2T_{i4}[D_0^4g]_0\ [D_0^2g_y]_0 + 1680(\sum_j\tau_{ij}T_{j4})[D_0^4g]_0\cdot g_{y,0}^2$$

$$+ 1120\rho_i^3T_{i3}[D_0^3g]_0\ [D_0^3g_y]_0 + 6720(\sum_j(\rho_i+\rho_j)\tau_{ij}T_{j3})[D_0^3g]_0\cdot g_{y,0}\cdot[D_0g_y]_0$$

$$+ 840\rho_i^4T_{i2}[D_0^2g]_0\ [D_0^4g_y]_0 + 20160(\sum_j\rho_i\rho_j\tau_{ij}T_{j2})[D_0^2g]_0\ [D_0g_y]_0^2$$

$$+ 10080(\sum_j(\rho_i^2+\rho_j^2)\tau_{ij}T_{j2})[D_0^2g]_0\cdot g_{y,0}\ [D_0^2g_y]_0$$

$$+ 20160(\sum_{jk}\tau_{ij}\tau_{jk}T_{k2})[D_0^2g]_0\ g_{y,0}^3 + 5040T_{i2}^2[D_0^2g]_0^2\cdot g_{yy,0}$$

$$+ 336\rho_i^5T_{i1}[D_0g]_0\ [D_0^5g_y]_0 + 20160(\sum_j\rho_i\rho_j(\rho_i+\rho_j)\tau_{ij}T_{j1})[D_0g]_0\cdot[D_0g_y]_0\cdot[D_0^2g_y]$$

$$+ 6720\Big(\sum_j(\rho_i^3+\rho_j^3)\tau_{ij}T_{j1}\Big)[D_0g]_0\cdot g_{y,0}\cdot[D_0^3g_y]_0$$

$$+ 40320\Big(\sum_{jk}(\rho_i+\rho_j+\rho_k)\tau_{ij}\tau_{jk}T_{k1}\Big)[D_0g]_0\ g_{y,0}^2\ [D_0g_y]_0$$

$$+ 6720T_{i1}T_{i3}[D_0g]_0\ [D_0^3g]_0\ g_{yy,0} + 20160\rho_iT_{i1}T_{i2}[D_0g]_0$$

$$[D_0^2g]_0\ [D_0g_{yy}]_0 + 10080\rho_i^2T_{i1}^2[D_0g]_0^2\ [D_0^2g_{yy}]_0$$

$$+ 20160\Big(\sum_j\tau_{ij}\ T_{j1}(2T_{i1}+T_{j1})\Big)[D_0g]_0^2\cdot g_{y,0}\ g_{yy,0}$$

$$+ 56\rho_i^6T_{i0}g_0\ [D_0^6g_y]_0 + 10080\Big(\sum_j\rho_i^2\rho_j^2\tau_{ij}T_{j0}\Big)g_0\cdot[D_0^2g_y]_0^2$$

$$+ 6720\Big(\sum_j\rho_i\rho_j(\rho_i^2+\rho_j^2)\tau_{ij}T_{j0}\Big)g_0\ [D_0g_y]_0\ [D_0^3g_y]_0$$

$$+ 1680\Big(\sum_j(\rho_i^4+\rho_j^4)\tau_{ij}T_{j0}\Big)g_0\ g_{y,0}\ [D_0^4g_y]_0$$

$$+ 40320\Big(\sum_{jk}(\rho_i\rho_j+\rho_j\rho_k+\rho_i\rho_k)\tau_{ij}\tau_{jk}T_{k0}\Big)g_0\ g_{y,0}\ [D_0g_y]_0^2$$

$$+ 20160\Big(\sum_{jk}(\rho_i^2+\rho_j^2+\rho_k^2)\tau_{ij}\tau_{jk}T_{k0}\Big)g_0\ g_{y,0}^2\ [D_0^2g_y]_0$$

$$+ 40320\Big(\sum_{jk\ell}\tau_{ij}\tau_{jk}\tau_{k\ell}T_{\ell0}\Big)g_0\ g_{y,0}^4 + 1680T_{i0}T_{i4}g_0\ [D_0^4g]_0\cdot g_{yy,0}$$

$$+ 6720\rho_iT_{i0}T_{i3}g_0\ [D_0^3g]_0\ [D_0g_{yy}]_0$$

$$+ 10080\rho_i^2T_{i0}T_{i2}g_0\cdot[D_0^2g]_0\ [D_0^2g_{yy}]_0$$

$$+ 20160\Big(\sum_j\tau_{ij}(T_{i2}T_{j0}+T_{i0}T_{j2}+T_{j0}T_{j2})\Big)g_0\ [D_0^2g]_0\ g_{y,0}\ g_{yy,0}$$

$$+ 6720\rho_i^3 T_{i0} T_{i1} g_0 \cdot [D_0 g]_0 \cdot [D_0^3 g_{yy}]_0$$

$$+ 40320\left(\sum_j \tau_{ij}(\rho_j T_{i0} T_{j1} + \rho_j T_{i1} T_{j0} + \rho_i T_{j0} T_{j1})\right) g_0 \cdot [D_0 g]_0 \cdot [D_0 g_y]_0 \cdot g_{yy,0}$$

$$+ 40320\left(\sum_j \tau_{ij}(\rho_i T_{i0} T_{j1} + \rho_i T_{i1} T_{j0} + \rho_j T_{i0} T_{j1})\right) g_0 \cdot [D_0 g]_0 \cdot g_{y,0} \cdot [D_0 g_{yy}]_0$$

$$+ 20160 T_{i0} T_{i1}^2 g_0 \; [D_0 g]_0^2 \cdot g_{yyy,0} + 840\rho_i^4 T_{i0}^2 g_0^2 \; [D_0^4 g_{yy}]_0$$

$$+ 10080\left(\sum_j \tau_{ij}(\rho_i^2 T_{j0} + 2\rho_j^2 T_{i0}) T_{j0}\right) g_0^2 \cdot [D_0^2 g_y]_0 \; g_{yy,0}$$

$$+ 20160\left(\sum_j \rho_i \rho_j \tau_{ij}(2T_{i0} + T_{j0}) T_{j0}\right) g_0^2 \; [D_0 g_y]_0 \cdot [D_0 g_{yy}]_0$$

$$+ 10080\left(\sum_j \tau_{ij}(\rho_j^2 T_{j0} + 2\rho_i^2 T_{i0}) T_{j0}\right) g_0^2 \cdot g_{y,0} \; [D_0^2 g_{yy}]_0$$

$$+ 20160\left(\sum_{jk} \tau_{ij}(2\tau_{jk} T_{i0} T_{k0} + 2\tau_{jk} T_{j0} T_{k0} + \tau_{ik} T_{j0} T_{k0} + \tau_{jk} T_{k0}^2)\right) g_0^2 \cdot g_{y,0}^2 \cdot g_{yy,0}$$

$$+ 10080 T_{i0}^2 T_{i2} g_0^2 \cdot [D_0^2 g]_0 \cdot g_{yyy,0} + 20160\rho_i T_{i0}^2 T_{i1} g_0^2 \cdot [D_0 g]_0 \cdot [D_0 g_{yyy}]_0$$

$$+ 3360\rho_i^2 T_{i0}^3 g_0^3 \; [D_0^2 g_{yy}]_0 + 20160\left(\sum_j \tau_{ij} T_{i0} T_{j0}^2\right) g_0^3 \cdot g_{yy,0}^2$$

$$+ 6720\left(\sum_j \tau_{ij}(3T_{i0}^2 + T_{j0}^2) T_{j0}\right) g_0^3 \; g_{y,0} \; g_{yyy,0}$$

$$+ 1680 T_{i0}^4 \; g_0^4 \cdot g_{yyyy,0}$$