Numerical Initial Value Problems for ODEs in Japan

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Abstract

Numerical solution for initial value problems of ordinary differential equations is a basic tool for scientific computations. At the same time it requires broad and deep mathematical theories for its analysis with respect to the order of accuracy, the stability, the implementation and so on. In the present paper we briefly sketch the development of the numerical solution in past decades with the emphasis on contributions of Japanese researchers.

1 Introduction

History of numerical solution of initial-value problem (IVP) of ordinary differential equations (ODEs) can trace back to the very beginning of the mathematical invention of ordinary differential equations. Since then, much contribution has been devoted to the theoretical as well as the practical development of the solution. In particular, among past decades the development can be said to have been as an accelerated one. The popularization of computational means in science and engineering has been prompting it, whereas the progress of computer capability, which is surely a fruit of modern science and engineering, opens a new aspect of the numerical solution. Henceforth a remarkable achievement has been obtained in numerical analysis of ordinary differential equations.

The present paper briefly surveys the development, and especially highlights contribution given by Japanese researchers to this field of study. Although their population is not so big as in Western countries, the numerical analysts community of Japan has made a considerable contribution.

1.1 IVP of ODEs and discrete variable methods

Throughout the present paper we will consider the following problem:

$$\frac{\mathrm{d}y}{\mathrm{d}x} = f(y) \quad (a < x < b), \qquad y(a) = y_0. \tag{1.1}$$

Here x is the independent variable, y the dependent variable (unknown function) which is a mapping from the interval $[a,b]$ to $\mathbb{R}^d$, f a given function from $\mathbb{R}^d$ to itself, and finally y_0 a given vector of $\mathbb{R}^d$. We adopt the *first order autonomous* formulation of ODEs, for other forms can be readily transformed into this.

Discrete variable method is a general class of numerical solution methods of (1.1). Upon the interval $[a,b]$ we take step-points $x_0(=a) < x_1 < \cdots < x_{n-1} < x_n < \cdots < x_N(=b)$, and try to generate a sequence of vectors $\{y_n\}$ $(n = 1, 2, \ldots, N)$ so that y_n is an approximation of the exact value $y(x_n)$. Basically the stepsize $h_n = x_{n+1} - x_n$ can vary with the index n, however theoretical results are often obtained under the assumption of constant stepsize $h_n = h$.

Other classes of methods, *e.g.,* a method approximating the solution with orthogonal polynomials, are surely considered, but the discrete variable method is most significant because of its readiness to produce general purpose software. Henceforth in the present survey we will focus on only the discrete variable method. Its main subclasses are *single-step* and *linear multistep* methods, while the *general linear methods* have been known to unify two subclasses. *Extrapolation*, which is powerful in many fields of numerical analysis, is also efficient in the implementation of discrete variable method for IVP of ODEs (1.1).

1.2 Historical background

Since the establishment of calculus in 17th century, the problem (1.1) has been known to be a basic mathematical expression for the physical phenomena including motion and/or variation. The brilliant success of the law of motion first described in *Principia* by I. Newton was to show that the motion of a planet around the sun which had been known to obey Kepler's law as a result of repeated astronomical observations could be fully explained with the differential equation of the two objects (two-body problem). However, since the three-body problem came to have no analytical solution, astronomical calculations needed to develop approximate numerical solutions of the equations of motion. Actually those who remained theirs names in the history of numerical analysis of IVP of ODEs, *e.g.,* J.C. Adams, F. Bashforth and F.R. Moulton, were originally astronomers.

On the other hand, as the simplest approximate solution of general IVP of ODEs is known as Euler's method, mathematicians were interested in such solutions, too. Since the time of Newton much more accurate methods than Euler's were known for the case of f in (1.1) *independent* of y but dependent of x. For example, the quadrature problem

$$\frac{\mathrm{d}y}{\mathrm{d}x} = f(x), \qquad y(x_0) = y_0$$

with solution

$$y(x) = y_0 + \int_{x_0}^{x} f(t)dt$$

has an approximate solution given by the recursion

$$y_n = y_{n-1} + h_{n-1} f\left(x_{n-1} + \frac{h_{n-1}}{2}\right).$$

The global error of the approximation is known to be bounded by Ch^2 (h is the maximum of h_i), while that of Euler's Ch. This motivated C. RUNGE to obtain higher order numerical solution of (1.1). It was a bit more than a hundred year ago that the classical paper of RUNGE appeared in *Mathematische Annalen* in 1895. Thus a very famous formula now called "the" Runge-Kutta method or the classical Runge-Kutta method was derived by W. KUTTA in 1901. Those who are interested in the historical investigation for the numerical solution up to the time of RUNGE and KUTTA can refer to the thesis [30] of D. TOURNÉS.

The invention as well as the rapid application of modern (electronic digital) computer fired further study of numerical solution of IVP. Its state-of-the-art up to the sixties can be seen in the classical textbook [7] of HENRICI. Since then, however, numerical solutions of IVP have achieved much progress. For instance, a systematic development of *implicit* Runge-Kutta methods, the sophisticated programming based on BDF (= backward differentiation formula) having stiff stability, order star concept smartly analyzing the stability feature by the application of complex function theory, and so on are recent big steps in numerical ODEs.

The progress in recent decades can be well written in the textbooks of J.D. LAMBERT, former [10] and new [11], [2] of J.C. BUTCHER, big two volumes [5] and [6] of E. HAIRER, S.P. NØRSETT and G. WANNER, and [1] of K. BURRAGE. Readers are recommended to refer to them to grasp the updated knowledge of numerical ODEs.

This survey paper, which will give a bird's eye view of this field of numerical analysis, will focus on the works carried out by Japanese researchers. Such contribution started in the early sixties to the numerical analysis community. However, several important papers were published only in Japanese, and, by virtue of some other additional reasons, their works are not necessarily known in other countries. The present author try to bridge the gap in this survey.

2 Runge-Kutta Methods

Single-step method class is represented by Runge-Kutta methods. As was written in the previous section, Runge-Kutta (RK in short) methods have a centennial history. However, it was only recently that some significant features of RK, *e.g.,* the non-existence of 5-stage 5th order (explicit) RK formula, were shown. This section will deal with the topics relevant to RK methods.

2.1 Explicit and implicit RKs

A Runge-Kutta formula for (1.1) is given by the following equations:

$$\left\{\begin{array}{rcl} Y_i &=& y_n + h_n \sum_{j=1}^{s} a_{ij} f(Y_j), \quad (i = 1, 2, \ldots, s) \\ y_{n+1} &=& y_n + h_n \sum_{i=1}^{s} b_i f(Y_i). \end{array}\right. \tag{2.1}$$

Here a natural number s is the number of stages of RK, a_{ij} and b_i the formula parameters. Associated with (2.1), we often introduce parameters c_i by

$$c_i = \sum_{j=1}^{s} a_{ij},$$

and adopt a matrix-vector notation given by

$$\begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array} \quad = \quad \begin{array}{c|c} \boldsymbol{c} & A \\ \hline & \boldsymbol{b}^T \end{array}, \tag{2.2}$$

where s-square matrix A, s-dimensional vectors $\boldsymbol{b}, \boldsymbol{c}$ stand for $(a_{ij}), (b_i), (c_i)$, respectively. The tableau given by (2.2) is often called the Butcher tableau of RK.

When the matrix A is strictly lower triangular ($a_{ij} = 0$ for $j \geq i$), RK is said to be *explicit*, while otherwise it is *implicit*. For example, the classical Runge-Kutta method is a 4-stage explicit one having the following Butcher tableau:

$$\begin{array}{c|cccc} 0 & & & & \\ 1/2 & 1/2 & & & \\ 1/2 & 0 & 1/2 & & \\ 1 & 0 & 0 & 1 & \\ \hline & 1/6 & 2/6 & 2/6 & 1/6 \end{array} \tag{2.3}$$

The *order of accuracy* of an RK is defined as follows. Suppose that in (2.1) we can obtain the exact value at nth step-point, *i.e.*, $y_n = y(x_n)$. The difference between the exact and the approximate values divided by the stepsize is called the *local truncation error* (LTE in short) and denoted by T_{n+1}, that is

$$T_{n+1} = \frac{1}{h_n} \left\{ y(x_{n+1}) - y(x_n) - h_n \sum_{i=1}^{s} b_i f(Y_i) \right\}. \tag{2.4}$$

The RK formula is said to be accurate of order p if for any sufficiently smooth exact solution $y(x)$ the estimation

$$T_{n+1} = O(h_n^p)$$

holds, but for a certain solution the estimation

$$T_{n+1} = O(h_n^{p+1})$$

does not hold. Thus the order of accuracy is an index how the formula can *locally* approximate the exact solution. At the same time, under a mild condition (for instance, Lipschitz continuity of f), it implies pth order of convergence of the approximate solution. That is, we obtain

$$\| y(x_n) - y_n \| = O(h^p) \quad \text{as} \quad h \to 0 \tag{2.5}$$

for any fixed x_n without the condition $y(x_n) = y_n$.

The notion of stability is crucial in RK, too. The assumption of the linear stability analysis is as follows: Suppose that we apply an RK to the linear test equation

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \lambda y, \qquad (\lambda \in \boldsymbol{C}, \quad \Re\lambda < 0) \tag{2.6}$$

with a certain initial value and a constant stepsize h. The RK then gives the recursion

$$y_{n+1} = R(z)y_n \tag{2.7}$$

where z stands for the complex variable $z = \lambda h$. In (2.7) the factor $R(z)$, which is called the *stability factor* of the RK, is generally a rational function of z with the coefficients determined with the formula parameters of (2.1). As a matter of fact, the identity

$$R(z) = \frac{\det(I - zA + z\boldsymbol{e}\boldsymbol{b}^T)}{\det(I - zA)} \tag{2.8}$$

holds, where $\boldsymbol{e}$ means the s-dimensional vector with unit entries.

Explicit RKs imply polynomial $R(z)$ of degree s, while implicit RKs yield rational $R(z)$. In both cases $R(z)$ is a p-th order approximation of $\exp(z)$ if the formula is accurate of p-th order. Furthermore the region

$$\mathcal{R} = \{z \in \boldsymbol{C}; |R(z)| < 1\}$$

is said to be the *region of absolute stability* of the formula. Generally speaking, the wider the region $\mathcal{R}$ is, the better the stability of the formula is. As its extreme, an RK is called to be A-stable when its region of absolute stability includes the left half-plane of $\boldsymbol{C}$.

2.2 Rooted tree analysis

As described in the previous subsection, the first interest for RK after the classical RK was to find higher order explicit RK formulae with less number of stages. Since the classical RK is a 4-stage fourth order formula, much effort had been devoted to show a 5-stage fifth order RK. The way of analysis is first to expand Y_i of (2.1) with respect to h_n in turn, and second to substitute them into the second of (2.1) so as to form the power series expansion of the approximate solution y_{n+1} with respect to h_n, and finally to compare the expansion with the Taylor series expansion of the exact solution $y(x_{n+1})$. The main tool of the execution is only the *chain rule* of differentiation, and we can obtain a system of simultaneous *nonlinear algebraic* equations of formula parameters a_{ij}, b_i, c_i. (This system is called the order conditions of the RK.)

However, the complexity of such system of equations increases almost exponentially as the required order and/or the number of stages increase. For instance, a 5-stage explicit RK which has 15 free parameters is required to satisfy 17 order conditions for fifth order. It was around 1963 that this question was negatively answered by three authors independently (Ceschino and Kuntzmann, Butcher, and Shanks) (see [5]). Among the process Butcher initiated a powerful means to derive both the Taylor series expansion of the exact

Table 2.1: Highest order attained by the number of stages

number of stages	1	2	3	4	5	6	7	8	9	10	≥ 10
highest order	1	2	3	4	4	5	6	6	7	7	$\leq s-2$

solution and the power series expansion of the numerical solution by applying the algebraic rooted tree theory. It not only made the order conditions transparent but also opened a broader exploratory way to more general class of numerical solutions, *e.g.,* implicit RKs, multiderivative methods, general linear methods and so on.

Hence, the theories of rooted tree and of B-series, associated with the former, are recognized to be efficient and applicable. They require, however, a long introduction, which cannot fit in the limitation of space of the present survey. Interested readers can refer to [2] and [5]. Here we give only the results obtained with the rooted tree analysis for RKs.

Theorem 2.1 *For explicit Runge-Kutta methods the following statements hold for the order of accuracy.*

(1) For $p \geq 5$ no method exists of order p with $s = p$ stages.

(2) For $p \geq 7$ no method exists of order p with $s = p + 1$ stages.

(3) For $p \geq 8$ no method exists of order p with $s = p + 2$ stages.

At present we can have Table 2.1 of the highest order versus the number of stages. The above restriction of the attainable order implies, on the other hand, that we have a certain freedom of formula parameters of RK of a specified number of stages even if it attains the highest order of accuracy. The freedom can be made use of to derive "optimized" formulae in several senses. For instance, S. HITOTUMATU pointed out in [8] that among 4-stage fourth order explicit RKs restricting the parameters so as to satisfy the conditions $a_{ij}, b_i, c_i \geq 0$ for all i and j, and $0 < c_2 \leq c_3 \leq c_4 \leq 1$ (the formula satisfying these can be said to be *monotone*), the classical RK is the only one. He further suggests that no monotone RK exists with stages greater than or equal to 5 and of the attainable order, but by now no proof is obtained.

Contrary to the explicit RK, the order result for implicit RK is very simple.

Theorem 2.2 *An s-stage implicit Runge-Kutta method can attain $(2s)$-th order, and the formula of the highest order is unique.*

As a matter of fact, when c_i's are taken as the roots of the shifted Legendre polynomial of degree s, the so-called *collocation* condition uniquely determines the other parameters, which result in the formula of $(2s)$th order. Since this determination has a close relationship with the Gauß-Legendre quadrature rule, the family of implicit RK is called the Gauß-Legendre type Runge-Kutta method, but recently more often referred to as Butcher-Kuntzmann method.

2.3 Optimization of RK parameters

In the previous subsection we mentioned the use of freedom of the formula parameters in explicit RKs. This means that an RK of an order of accuracy with the specified number of stages can be *optimized* in a certain sense. M. TANAKA has systematically developed such optimization for both explicit and implicit RKs.

He adopted five criteria for RK formulae. First is that for the truncation error. As shown in (2.4), the local truncation error of an s-stage p-th order RK is expressed in

$$\left\{ \begin{array}{rcl} T_{n+1} & = & g_p h_n^p + O(h^{p+1}), \\ g_p & = & \displaystyle\sum_{l=1}^{L_p} \alpha_{pl} g_l(y_n), \end{array} \right. \tag{2.9}$$

where $g_l(y_n)$ is the so-called *elementary differential* of f of order p appearing in the tree analysis of RKs, and coefficients α_{pl} depend only on the formula parameters. When the solution of p-th order conditions is taken, the coefficients can be expressed in the free formula parameters. Thus two quantities

$$\left\{ \begin{array}{rcl} A_{p1} & = & \displaystyle\sum_{l=1}^{L_p} |\alpha_{pl}| \\ A_{p2} & = & \displaystyle\sum_{l=1}^{L_p} \alpha_{pl}^2 \end{array} \right. \tag{2.10}$$

reflect the LTE feature of the formula. The less A_{p1} or A_{p2} becomes, the better the formula has its LTE feature.

Second, he introduces two measures for the linear stability of the formula. The area A_e of the following region $\mathcal{R}_e$ in $\boldsymbol{C}$, which is referred to the *effective region* of absolute stability, is one criterion.

$$\mathcal{R}_e = \text{simply connected region of} \quad \bar{\mathcal{R}} \cap \boldsymbol{C}^- \quad \text{including the origin}$$

Another is the positive number α satisfying

$$[-\alpha, 0] = \boldsymbol{R} \cap \mathcal{R}_e$$

That is, $-\alpha$ indicates the left-most point of the interval of absolute stability.

Third criterion R corresponds to the *rounding error* of the formula. Since serious lack of significant digits may occur in a single step integration of RK due to the big coefficients a_{ij} and b_i in magnitude, the quantity

$$R = \sum_{i,j} |a_{ij}| + \sum_i |b_i| \tag{2.11}$$

can stand for the criterion. In particular, when R is small, an explicit RK is expected to make the rounding error smaller.

Applying the criteria described above, TANAKA with the collaboration of many coworkers developed an automated computer program to examine the feature of a given combination of

the formula parameters of RK. Furthermore, utilizing the nonlinear optimization technique, they systematically investigated the optimized parameters of explicit RKs of up to 8-th order. Considering A_{p1} and A_{p2} in (2.10), and the area of $\mathcal{R}_e$ and α in the stability criteria, they also examined the feature of some implicit RKs. Their works are partially reported in [28], which is not known internationally because of its publication in Japanese.

2.4 'Limiting formula' of explicit RK

Another application of the freedom of the formula parameters in explicit RKs is their 'limiting formula'. H. TODA ([29]) carefully studied the solution of the order conditions of 5-stage *fourth order* explicit RK including free parameters, and, taking the limit $c_2 \to 0$ or $c_4 \to 1$, derived two formulae being of fifth order. For example, in the case of $c_2 \to 0$ the limiting formula can be obtained by observing that the substitution of the formal solution into the combinations $b_1 + b_2, a_{i1} + a_{i2}, b_2 c_2, a_{i2} c_2$ $(i = 3, 4, 5)$ yields no factor of $1/c_2$ into them. Thus, by rewriting

$$b_1 f(Y_1) + b_2 f(Y_2) = (b_1 + b_2) f(Y_1) + b_2 c_2 \left(f(Y_2) - f(Y_1) \right) / c_2$$

and taking the limit

$$\lim_{c_2 \to 0} \left(f(Y_2) - f(Y_1) \right) / c_2 = h_n f' \cdot f,$$

we arrive at

$$b_1' f(Y_1) + \bar{b}_2 h_n f'(Y_1) \cdot f(Y_1)$$

in place of the sum $b_1 f(Y_1) + b_2 f(Y_2)$. Further similar algebraic computations can lead to *a 5-stage fifth order RK* still remaining c_3 and c_4 free, at the expense of the introduction of the derivative f' (the Jacobian matrix of f).

In this way H. TODA and H. ONO have developed 5-stage fifth order, 6-stage sixth order, 7-stage seventh order and 8-stage seventh order limiting RK formulae ([29, 19, 17, 20, 21, 18]). There they also discuss the optimization of the limiting formulae by using the remained free parameters, and study explicit RK of numerically same order as the corresponding limiting formula without the derivative evaluations. It is carried out by taking advantage of the fact that the significant digits provided by the derivative term need not so many as those from the f-evaluations in actual numerical computations. Hence the derivative may be effectively approximated with the difference quotient.

Stepping forward to the direction of introduction of the second derivative of the solution $y(x)$ of (1.1) into numerical scheme, we arrive at a generalization of the Runge-Kutta methods involving the second derivative. Succeeding the works of H. SHINTANI [26, 27], who considered some special type of single-step methods utilizing the second derivative, T.

MITSUI [15] proposed the following scheme of Runge-Kutta type.

$$\left\{\begin{array}{rcl} Y_i &=& y_n + h_n\sum_{j=1}^{s} a_{ij} f(Y_j) + h_n^2\sum_{j=1}^{t} b_{ij} g(Z_i), \quad (i=1,2,\ldots,s) \\ Z_i &=& y_n + h_n\sum_{j=1}^{s} c_{ij} f(Y_j) + h_n^2\sum_{j=1}^{t} d_{ij} g(Z_i), \quad (i=1,2,\ldots,t) \\ y_{n+1} &=& y_n + h_n\sum_{i=1}^{s} \mu_i f(Y_i) + h_n^2\sum_{i=1}^{t} \nu_i g(Z_i). \end{array}\right. \tag{2.12}$$

Here $g(y)$ denotes the second derivative of y with respect to x, *i.e.*, $g(y) = f'(y)f(y)$. Developing a theory for the power series expansion of (2.12) in h_n with the Bell polynomials, which is essentially equivalent to the rooted tree analysis, MITSUI examined the attainable order of the explicit formulae in the case of $s=1, t=1$ to $s=1, t=4$. Other aspects, *e.g.* linear stability analysis, embedded formulae and so on, are however left in an interrupted state.

Another stepping to the direction is to introduce the evaluation of the Jacobian of f into the stage value of RK. ROW method is its systematical realization. That is to say, instead of (2.1), the scheme is expressed into the following:

$$\left\{\begin{array}{rcl} y_{n+1} &=& y_n + h_n\sum_{i=1}^{s} b_i k_i, \\ (I - h_n\gamma J)k_i &=& f\left(y_n + h_n\sum_{j=1}^{i-1} a_{ij}k_j\right) + h_n J\sum_{j=1}^{i-1}\gamma_{ij}k_j \end{array}\right. \tag{2.13}$$

Here J means the evaluated Jacobian of f at y_n. The scheme (2.13) is known to be effective for stiff problems.

2.5 Pseudo-Runge-Kutta or two-step Runge-Kutta

To improve the performance of RK method in the viewpoint of the correlation of the number of stages and the order, we think of an introduction of the back values of step-point. Suppose that the stepsize is constant as h and we have the backvalues $y_n, y_{n-1}, \ldots$. M. NAKASHIMA [16] considered the *pseudo-Runge-Kutta* method given by the following:

$$\left\{\begin{array}{rcl} Y_0 &=& y_{n-1} \\ Y_i &=& y_n + a_i(y_n - y_{n-1}) + h\sum_{j=0}^{s} a_{ij} f(Y_j) \\ y_{n+1} &=& y_n - b_0(y_n - y_{n-1}) + h\sum_{i=0}^{s} b_i f(Y_i) \end{array}\right. \tag{2.14}$$

Under the constant-stepsize integration, we can keep the off-step values $y_{n-1}(=Y_0)$ and $f(Y_0)$. Henceforth, if we can raise up the attainable order of the pseudo-RK from that of the usual RK of the same number s of stages, the performance is improved without extra costs

of the function evaluation for f. Actually NAKASHIMA showed that the formulae (2.14) of $s = 2, 3$ and 4 can attain fourth, fourth and fifth, respectively, order, and obtained some pairs of embedded pseudo-RK.

Similar idea as in NAKASHIMA has also been developed in [3, 4] under the name of 'two-step Runge-Kutta'.

2.6 Symplectic integration

Several special classes of Runge-Kutta or single-step methods have been attracting attentions of both theorists and practitioners. A significant one is numerical *symplectic* integrators, which can preserve the symplectic structure of Hamiltonian dynamical systems. Let Ω be a domain in the oriented Euclidean space $\mathbb{R}^{2d}$, which is the totality of the state points $(\boldsymbol{p}, \boldsymbol{q}) = (p_1, \ldots, p_d; q_1, \ldots, q_d)$. In classical mechanics, the $\boldsymbol{q}$ variables are called the *generalized coordinates,* while the $\boldsymbol{p}$ variables the conjugated *generalized momenta.* If H is a sufficiently smooth real function defined on Ω, the Hamiltonian system of differential equations with Hamiltonian H is given by

$$\frac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}t} = -\frac{\partial H}{\partial \boldsymbol{q}}, \quad \frac{\mathrm{d}\boldsymbol{q}}{\mathrm{d}t} = \frac{\partial H}{\partial \boldsymbol{p}}, \tag{2.15}$$

or in a vector form as

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} \boldsymbol{p} \\ \boldsymbol{q} \end{pmatrix} = J_{2d}\nabla H, \quad \text{where} \quad J_{2d} = \begin{bmatrix} 0 & -I_d \\ I_d & 0 \end{bmatrix} \tag{2.16}$$

and ∇ means the gradient operator. Either of the above equations is called the Hamilton's *canonical* equation with H, which usually corresponds to the total mechanical energy.

For $t \in \mathbb{R}$, φ_t stands for the flow of the system (2.15). That is, φ_t is a transformation on Ω into itself (as a matter of fact, a one-parameter group of diffeomorphisms) so that for $(\boldsymbol{p}^0, \boldsymbol{q}^0) \in \Omega$, $(\boldsymbol{p}, \boldsymbol{q}) = \varphi_t(\boldsymbol{p}^0, \boldsymbol{q}^0)$ is the value at t of the solution of (2.15) with the initial value $(\boldsymbol{p}^0, \boldsymbol{q}^0)$ at $t = 0$. And the remarkable property of this Hamiltonian flow is that it preserves the symplectic structure on Ω. Furthermore, if Ω is simply connected, then the converse is also true; a symplectic differential system is a Hamiltonian system.

Let ω^2 be the differential 2-form on Ω given by $\sum_i dp_i \wedge dq_i = d\boldsymbol{p} \wedge d\boldsymbol{q}$, then the transformation φ_t is symplectic if and only if

$$d\boldsymbol{p} \wedge d\boldsymbol{q} = d\boldsymbol{p}^0 \wedge d\boldsymbol{q}^0 \tag{2.17}$$

for $(\boldsymbol{p}, \boldsymbol{q}) = \varphi_t(\boldsymbol{p}^0, \boldsymbol{q}^0)$. Here $\wedge$ denotes the symbol of the exterior product of forms. The symplecticness of a Hamiltonian system geometrically implies its preservation of the *oriented volume* in $\mathbb{R}^{2d}$.

Suppose the single-step discrete variable methods applied to the canonical equation (2.15). Let $(\boldsymbol{p}^n, \boldsymbol{q}^n)$ stands for the numerical approximation at $t_n = nh$ with the step-size h for the value $(\boldsymbol{p}(t_n), \boldsymbol{q}(t_n))$ of a solution of the equation. Then a single-step method is associated with a mapping ψ_h given by

$$(\boldsymbol{p}^{n+1}, \boldsymbol{q}^{n+1}) = \psi_h(\boldsymbol{p}^n, \boldsymbol{q}^n). \tag{2.18}$$

The single-step transformation ψ_h, which is assumed to be a smooth function with respect to h, should be an approximation of the transformation φ_h of the intrinsic flow at $t = h$.

Since the equation (2.16) can be regarded as a system of ODEs, an application of RK (2.1) with the Butcher tableau (2.2) to it yields

$$\boldsymbol{P}_i = \boldsymbol{p}^n + h\sum_{j=1}^{s} a_{ij}\boldsymbol{f}(\boldsymbol{P}_j, \boldsymbol{Q}_j), \quad \boldsymbol{Q}_i = \boldsymbol{q}^n + h\sum_{j=1}^{s} a_{ij}\boldsymbol{g}(\boldsymbol{P}_j, \boldsymbol{Q}_j), \qquad (i = 1, \ldots, s) \tag{2.19}$$

$$\boldsymbol{p}^{n+1} = \boldsymbol{p}^n + h\sum_{i=1}^{s} b_i\boldsymbol{f}(\boldsymbol{P}_i, \boldsymbol{Q}_i), \quad \boldsymbol{q}^{n+1} = \boldsymbol{q}^n + h\sum_{i=1}^{s} b_i\boldsymbol{g}(\boldsymbol{P}_i, \boldsymbol{Q}_i), \tag{2.20}$$

where $\boldsymbol{f}$ and $\boldsymbol{g}$ mean the right-hand side vectors in (2.15).

A remarkable condition under which the RK is symplectic was given by F. M. Lasagni, J. M. Sanz-Serna and Yu. B. Surius independently (see [24]).

Theorem 2.3 *Let B denote the diagonal matrix* $\mathrm{diag}(b_1, b_2, \ldots, b_s)$, *and define the matrix M as*

$$M = BA + A^T B - \boldsymbol{b}\boldsymbol{b}^T.$$

Suppose that none of b_i's vanishes (the condition is often referred as the non-redundancy of the stages), then the RK scheme is symplectic if and only if the identity $M = 0$ holds.

Implications of the Theorem for the order conditions of RK through the rooted tree analysis, which was carried out by Sanz-Serna and Abia, was also given by the group of the present author independently ([22, 23, 14]). And some of the concrete examples of symplectic RK formula have been studied by S. Maeda together with the topic of preservation of quadratic first integral of linear system via RK ([12]).

Although RK is the representative class of single-step methods, another alternative approach is possible for symplectic numerical methods. Basic idea is 'splitting' (or fractional step) and 'composition' of a numerical scheme. For instance, let $\psi_h^{[B]}$ denote the flow by the simplest ($s = 1$) Gauß-Legendre RK, and consider the composed flow

$$\Psi_h = \psi_{\theta_1 h}^{[B]} \cdot \psi_{\theta_0 h}^{[B]} \cdot \psi_{\theta_1 h}^{[B]}$$

where the parameters θ_0 and θ_1 satisfying $\theta_0 + 2\theta_1 = 1$ are selected to make the approximation order as many as possible. This type of schemes has been systematically developed through the concept of the Baker-Campbell-Hausdorff formula. H. Yoshida ([34]), who is basically an astrophysicist again, can be credited with the pioneer of this direction. Details may be referred in [24].

3 Linear Multistep Methods

A linear multistep method (LMM, in short) is a discrete variable method for (1.1) to give an approximation y_{n+k} at x_{n+k} making use of the back values $y_{n+k-1}, \ldots, y_n$ at the equidistant step-points in a linear manner. That is, y_{n+k} is calculated through the formula

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h\sum_{j=0}^{k} \beta_j f_{n+j}, \tag{3.1}$$

where $f_j = f(y_j)$ and α_j and β_j are the formula parameters. The number k stands for the number of steps of the LMM, and the case $\beta_k = 0$ is called explicit, while otherwise implicit. The first and the second characteristic polynomials of (3.1) are given as

$$\rho(\zeta) = \sum_{j=0}^{k} \alpha_j \zeta^j, \qquad \sigma(\zeta) = \sum_{j=0}^{k} \beta_j \zeta^j, \tag{3.2}$$

respectively.

All the details of LMM are found in the aforementioned textbooks on numerical ODEs. Thus here we focus on contributions of Japanese researchers for this topic of study.

3.1 Milne's device and its modification

One of the features of LMM is a cheap and efficient way for *a posteriori* error estimation. It is usually carried out as follows. Since an LMM integrates one step by taking an explicit and implicit formula pairs of the same order as the predictor and the corrector, respectively, (hence it is called a PC method) assume that the k-step predictor LM formula with $\{\alpha_j^*, \beta_j^*\}$ of m-th order is associated with the corrector LM formula of $\{\alpha_j \beta_j\}$ and of the same order. (Note that some of α_j and β_j of small index are assumed to be zero to make the corrector formally of the same number of steps.) Under the so-called *localization assumption* ($y_{n+j} = y(x_{n+j}),\ j = 0, 1, \ldots, k-1$), the predicted value y_{n+k}^P and the corrected value y_{n+k}^C have the error terms expressed with

$$y(x_{n+k}) - y_{n+k}^P = C^* h^{m+1} y^{(m+1)}(x_n) + O(h^{m+2}), \tag{3.3}$$

$$y(x_{n+k}) - y_{n+k}^C = C h^{m+1} y^{(m+1)}(x_n) + O(h^{m+2}). \tag{3.4}$$

Here C^* and C, called the local error-constant, are rational numbers and the former is bigger than the latter in magnitude. Then, what W. E. Milne was found is that, by neglecting higher order terms, the local error of the corrector can be estimated as

$$y(x_{n+k}) - y_{n+k}^C \approx \frac{C}{C^* - C} \left(y_{n+k}^C - y_{n+k}^P \right). \tag{3.5}$$

Then, what follows when we remove the localization assumption? M. Iri [9] studied the topic, and obtained that the estimation (3.5) is modified as

$$y(x_{n+k}) - y_{n+k}^C \approx \frac{C}{C^* - \dfrac{\sigma^*(1)}{\sigma(1)} C} \left(y_{n+k}^C - y_{n+k}^P \right). \tag{3.6}$$

Here $\sigma^*(\zeta)$ and $\sigma(\zeta)$ stand for the second characteristic polynomial of the predictor and of the corrector, respectively. It means when $\sigma^*(1)$ and $\sigma(1)$ differs each other, (3.6) will give more precise estimates than (3.5). Unfortunately in the Adams-type pairs of predictor and corrector this is not the case.

3.2 Urabe's method

To derive an LMM of (3.1), M. URABE [31] adopted a way different from the traditional one. The Adams-type methods have the first characteristic polynomial as $\rho(\zeta) = \zeta^k - \zeta^{k-1}$. Through an analysis of the magnitude of error constants, he took $\rho(\zeta) = \zeta^{k-1} - \zeta^{k-2}$, while $\sigma(\zeta) = \sum_{j=0}^{k} \beta_j \zeta^j$. This unbalance appears curious, however the error constant really turns out to be smaller. For instance, in the 5-step method case, he gave the fifth-order implicit formula

$$y_{n+4} - y_{n+3} = \frac{h}{720}\left(-19f_{n+5} + 346f_{n+4} + 456f_{n+3} - 74f_{n+2} + 11f_{n+1}\right), \tag{3.7}$$

whose error term is given as

$$\frac{11}{1440}h^6 y^{(6)}(\xi).$$

The corresponding Adams-type explicit and implicit formulae are

$$y_{n+5} - y_{n+4} = \frac{h}{720}\left(1901f_{n+4} - 2774f_{n+3} + 2616f_{n+2} - 1274f_{n+1} + 251f_n\right), \tag{3.8}$$

$$y_{n+5} - y_{n+4} = \frac{h}{720}\left(251f_{n+5} + 646f_{n+4} - 264f_{n+3} + 106f_{n+2} - 19f_{n+1}\right), \tag{3.9}$$

whose error terms are

$$\frac{95}{288}h^6 y^{(6)}(\xi') \quad \text{and} \quad -\frac{3}{160}h^6 y^{(6)}(\xi''),$$

respectively. Note that the error constants reduce their magnitude by one digit for the explicit Adams, implicit Adams and Urabe in this order.

Of course an implementation of Urabe's formula (3.7) calls an attention, for it utilizes the $(n+5)$-th step evaluation of f in the right-hand side which passes over the left-hand side evaluation ($(n+4)$-th step). Henceforth he combined it with the explicit Adams-type formula (3.8) in a PC mode. That is to say, employing (3.8) to give a predicted value y^*_{n+5}, we substitute it in the right-hand side of (3.7) to calculate a corrected value y_{n+4}. The process is repeated until a sufficiently accurate approximation is obtained for $y(x_{n+4})$. Then one-step forwarding is carried out. URABE and his group succeeded in numerical computations of autonomous oscillation of the van der Pol equation by this PC method ([33]).

Later, Y. SHINOHARA [25] systematically analyzed Urabe's method and to prove its zero-stability. As a matter of fact, he named the method after URABE, who unfortunately passed away in 1975 at the age of 62.

In his paper of 1970 ([32]), URABE further developed his idea to employ the second derivative evaluation in LMM. As in **2.4**, let $g(y)$ stand for the second derivative of y with respect to x. In the actual situation it can be called a single-step method, but he derived the following PC pair. The predictor is

$$y_{n+2} - 32y_{n+1} + 31y_n = -h\left(16f_{n+1} + 14f_n\right) + h^2\left(4g_{n+1} - 2g_n\right), \tag{3.10}$$

while the corrector

$$y_{n+1} - y_n = \frac{h}{240}\left(11f_{n+2} + 128f_{n+1} + 101f_n\right) + \frac{h^2}{240}\left(-3g_{n+1} - 40g_{n+1} + 13g_n\right). \qquad (3.11)$$

The predictor is of fifth order with the error term

$$\frac{1}{90}h^6 y^{(6)}(\xi),$$

while the corrector of sixth-order with

$$\frac{1}{9450}h^7 y^{(7)}(\xi').$$

He showed its convergence as well as a step-size controlling rule. An absolute stability analysis was carried out by MITSUI [13]. In the present author's view, Urabe's method has not, however, been studied enough, in particular for a general-purpose implementation.

4 Concurrent works

In the present author's community of Japanese, we can refer to the following names and works other than those already mentioned in the previous sections. Their distribution reflects on the present topics in the community.

T. Koto (Tokyo)

Starting with numerical analysis of ODE cases, he is currently devoting himself for the stability analysis of RK applied to delay differential equations (DDEs). It includes not only the natural RKs but also the quadrature-type RKs. He deals with stability for DDEs of both scalar and system cases, employing the Lyapunov functional method or the positive real lemma of the linear system theory.

K. Kubota (Tokyo)

He is interested in the self-validated numerical solution of IVP of ODEs applying the fast automatic differentiation (FAD). FAD and its implementation are crucial for numerical ODEs when they come from industrial problems like as in chemical engineering.

M. Murofushi (Sagamihara)

He is dealing with the Richardson extrapolation as well as its application to numerical ODEs, and proposed a stopping rule in conjunction with the machine epsilon.

K. Ozawa (Sendai)

He is interested in the parallel solution of IVP of ODEs, and developing such solutions via the waveform relaxation, the block PC methods and the parallel RKs. Some test examples were carried out by him on computers of the parallel architecture. He is also developing an unconventional type of RKs.

Y. Saito (Gifu)

Starting with stability analysis for numerical discrete-variable solution of stochastic differential equations (SDEs), he is interested in numerical solutions of stochastic PDEs in their applications to physical phenomena, modelled with, *e.g.,* the KPZ equation.

Ch. Suzuki (Fukuroi)

He is studying a class of the general linear methods, and derived some new formulae possessing a good stability as well as accuracy. Furthermore, he developed applications of such class to Volterra-type integro-differential equations, which may in some case include a delay.

The present author (Nagoya)

Other than the topics previously mentioned in the present article, the present author is interested in

- numerical solutions and their stability of SDEs,
- numerical solutions and their stability of DDEs,
- finite differencing of PDEs and its parallelization in the time-integration,
- finite difference solution of several soliton equations

in collaboration with a number of colleagues.

As a concluding remark, the present author feels an academic achievement of our community in Japan, but also likes to point out that there is still a lack of industrial applications. The scientific and engineering needs, not only domestic bu also international, for numerical computation require more sophisticated and robust solutions of ODEs and of their related. Actually there are some software to cope with the problem. We are expected to contribute more to the problem.

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