THE DIRECT NUMERICAL INTEGRATION METHODS FOR LARGE SCALE ORDINARY DIFFERENTIAL EQUATIONS

— Evaluation and Proposal of Numerical Integration Methods —

by

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Abstract

This paper deals with the direct numerical integration methods for large scale differential equations. A method to evaluate the numerical integration in s-plane and z-plane is given, and several integration operators are evaluated by using the method.

Next, new direct numerical integration methods for large scale differential equations are proposed on the basis of the results obtained above, and numerical computations are made by using the electronic digital computer programs in terms of the proposed methods.

After the computations, the evaluation method of numerical integration is found to be reasonable, and the proposed methods of direct integration to be suitable for large scale problems.

1. Introduction

In recent engineering fields, analysis of large scale structures or industrial systems has been very important. As a method

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obtaining approximate solutions of governing equations corresponding to physical systems, especially large scale structures or industrial systems, the finite element method has been quite remarkably developed.[1],[2] This finite element method is a one which discretizes the system being of interest and can be adaptable to both linear and nonlinear systems. In the finite element method analysis, the equations which govern the behavior of the systems have to be usually solved in time domain to obtain the dynamic responses of linear systems or the step-by-step responses of nonlinear systems. The problems which arise in the analysis are generally characterized by large scale, sparse, and real symmetric properties in coefficient matrices of differential equations. Particularly, because of largeness of the order of matrices, their eigen-values distribute widely in eigen-plane, and this may come to unstable phenomena in numerical integration. To avoid these unstable phenomena in numerical computations of practical problems, computational times are excessively required. Therefore, an efficient and stable method is eagerly desired to be developed[3] obtaining an approximate solution of differential equations of the problems in time domain (a numerical integration method).

Various methods of numerical integration for ordinary differential equations have been studied.[4]∿[20] But it is generally difficult to know the best method in applying the numerical integration to practical problems, because evaluation of precision and stability of the method can not be easily and systematically done, and furthermore differential equations dealt with in practice vary from several orders to several thousand orders in their size.

From the point of view described above, this paper concerns the following studies; (1) Proposing a method to systematically evaluate the basic characteristics of the numerical integration method and evaluating typical existing numerical integration methods (integration operators) based on the proposed method, (2) Proposing new numerical integration methods for large scale ordinary differential equations (particularly, for second order simultaneous ordinary matrix differential equations) on the basis of the item (1).

2. Evaluation of Numerical Integration Method for Ordinary Differential Equations

M ; mass matrix (MxM) **C** ; damping matrix (MxM)

K ; stiffness matrix (MxM) **A** ; system matrix (MxM)

B ; coefficient matrix corresponding to forcing function (2MxM)

$\mathbf{P}_{pp}$; pth diagonal Padé approximation function

$\mathbf{R,S,T,U,V,}$; working matrices $\mathbf{y}$; state vector (2Mx1)

$\mathbf{x}, \dot{\mathbf{x}}, \ddot{\mathbf{x}}$; displacement, velocity, and acceleration vectors (Mx1)

$\mathbf{f}$; forcing vector $\mathbf{u,v,w}$; working vectors

$F(s\tau)$; characteristic root of integration operator

c_i ; constant concerning with integration operator

l ; interpolation order of forcing function

p ; approximation order of diagonal Padé approximation function

τ ; mesh size in numerical computation

Vectors and matrices containing the subscript n denote the ones at time $n\tau$.

In this chapter, a method to evaluate the numerical integration method for ordinary differential equations is given, and then typical existing numerical integration methods are evaluated on the basis of the method described above. In the case of dealing with a non-linear system, the equation is assumed to be approximated to the piece-wise linear system, and evaluation of numerical integration methods is done from a view point of function approximation of $\exp(s\tau)$ which is the basic solution of a linear system.

2.1 Preparations and Criteria for Evaluation of Numerical Integration Methods

A linear simultaneous ordinary differential equation can generally be written in the form of

$$\dot{\mathbf{y}} = \mathbf{A}\mathbf{y} + \mathbf{B}\mathbf{f} \qquad \mathbf{y}(0) = \mathbf{y}_0 \tag{1}$$

using a state vector $\mathbf{y}$. Now, a forcing function $\mathbf{f}(t)$ during time interval $n\tau \sim (n+1)\tau$ is assumed to be written as

$$\mathbf{f}_n(n\tau+\eta) \equiv \mathbf{f}_n(\eta) = \sum_{i=0}^{l} \frac{\eta^i}{i!} \mathbf{f}_n^{(i)} \tag{2}$$

by using the lth polynomial function of a discrete sequence $\{\mathbf{f}_n\}$, where $\mathbf{f}_n^{(i)}$ indicates the i th derivative of $\mathbf{f}(n\tau)$ at time $n\tau$. Then, relationship between the state vectors $\mathbf{y}_{n+1}$ and $\mathbf{y}_n$ at times $(n+1)\tau$ and $n\tau$ in Eq. (1) is obtained as

$$\mathbf{y}_{n+1} = e^{\mathbf{A}\tau}\mathbf{y}_n + e^{\mathbf{A}(n+1)\tau} \int_{n\tau}^{(n+1)\tau} e^{-\mathbf{A}\eta}\mathbf{B}\mathbf{f}_n(\eta)\, d\eta \,. \tag{3}$$

Substituting Eq. (2) into Eq. (3) and integrating the equation, we obtain

$$\mathbf{y}_{n+1} = e^{\mathbf{A}\tau}\mathbf{y}_n + \sum_{i=0}^{l}\left\{\left(e^{\mathbf{A}\tau} - \mathbf{I}\right)\mathbf{A}^{-(i+1)} - \sum_{j=0}^{i-1}\frac{\tau^{i-j}}{(i-j)!}\mathbf{A}^{-(i+1)}\right\}\mathbf{B}\mathbf{f}_n^{(i)} \quad (4)$$

This is the difference representation of Eq. (1) and is the basic equation to compute numerical integration of the differential equation by an electronic digital computer. We call $e^{\mathbf{A}\tau}$ a state transition matrix and it can be calculated by its definition

$$e^{\mathbf{A}\tau} = \sum_{i=0}^{\infty}\frac{1}{i!}\mathbf{A}^i\tau^i \quad . \quad (5)$$

The second term of the right hand side of Eq. (4) is the numerical integration term corresponding to a forcing function. If $\mathbf{f}_n^{(i)}$ is assumed to be

$$\mathbf{f}_n^{(i)} = \nabla^i\mathbf{f}_n / \tau^i \quad (6)$$

by the difference of a data sequence $\{\mathbf{f}_n\}$, difference equation (4) can compute a solution from an initial condition $\mathbf{y}_0$ by means of a step-by-step method. This gives the exact solution to every computational mesh size τ.

Now let us consider the characteristics of difference representation (4). Here without loss of generality, an arbitrary value s instead of $\mathbf{A}$ in eigen-plane of $\mathbf{A}$ which has distinct eigenvalues and a scalar value b instead of $\mathbf{B}$ can be used in Eq. (4). Consequently, Eq. (4) is simply written as

$$y_{n+1} = e^{s\tau}y_n + \sum_{i=0}^{l}\left(q_i/\tau^i\right) f_n^{(i)} \quad (4)'$$

where, q_i is

$$q_i = \left\{\left(e^{s\tau} - 1\right)/s^{i+1} - \sum_{j=0}^{i-1}\tau^{i-j}/\left((i-j)!\,s^{j+1}\right)\right\} b \quad . \quad (7)$$

Z transformation of difference equation (4)' gives a relation

$$Y(z) = H(z, s\tau)\,F(z) \quad (8)$$

between a forcing function $F(z)$ and a solution $Y(z)$, where $H(z, s\tau)$ is given by

$$H(z, s\tau) = \sum_{j=0}^{l} \frac{1}{\tau^i} q_i (z-1)^i / (z - e^{s\tau}). \tag{9}$$

Eq. (9) is the transfer function related to z operator containing a parameter $s\tau$. If $F(z)$ is applied to Eq. (8), the solution $Y(z)$ of the differential equation having a characteristic root s for every time mesh τ is obtained. Because of the reasons described above, the transfer function $H(z, s\tau)$ and the difference equation which is equivalent to it, will be generically called an integration operator (or simply an operator). When the denominator and the numerator of the transfer function must be distinguished, we call them a state transition operator and a forcing operator, respectively.

Let the function derived from the transition operator be zero, that is,

$$z - e^{s\tau} = 0 \tag{10}$$

This is called the characteristic equation of the integration operator, and the root $e^{s\tau}$ is called a characteristic root or a pole. The exponential function is the exact mapping which transforms a differential equation into a difference equation. But in practical numerical computations, because of the reasons which will be described in section 2.2, an approximation function $F(s\tau)$ to exp. function is used as a state transition operator. Consequently, in the case of evaluating the integration operator, it is reasonable to refer the characteristics of exp. function as a criterion.

The criterion used herein is as follows:
(Criterion); A value on the imaginary axis in -plane is transformed into

$$z = e^{i\omega\tau} = 1 \angle \omega\tau, \quad s = i\omega \tag{11}$$

in z-plane by exp. function. This is the mapping from an $i\omega\tau$ in $s\tau$-plane into a value on the unit circle in z-plane. Accordingly, the operator $F(i\omega\tau)$ must enoughly approximate the characteristics of Eq. (11).

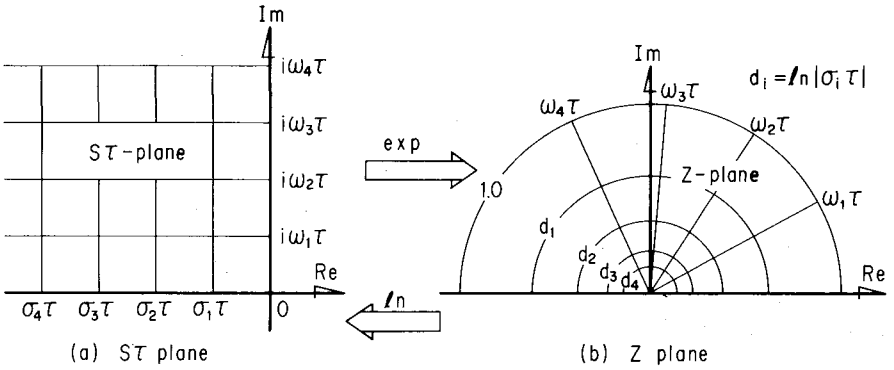


Fig. 1. Mapping relationship between $s\tau$-plane and z-plane

2.2 Evaluation Method for Numerical Integration Method

Computing a differential equation based on the Eqs. (4) and (5), the solution can exactly be obtained. But the computation of ${}_e\mathbf{A}^{\tau}$ in terms of the right hand side of Eq. (5) needs so huge amount of treatments and memory capacity that this is not practical. Therefore, in general, the approximation function is adopted instead of exponential function. We can obtain

$$R_p(s\tau)\,y_{n+1} = -\sum_{i=1}^{p} R_{p-i}(s\tau)\,y_{n+1-i} + \sum_{j=0}^{l} T_j(s\tau)\,f_{n+j} \tag{12}$$

by means of the approximation function $F(s\tau)$ from Eq. (1) in such a way that one obtained Eq. (4) by means of $e^{s\tau}$ from Eq. (1) having a characteristic root s. Z transformation of Eq. (12) reduces to the relation

$$Y(z) = [\,Q(z,\ s\tau)/P(z,\ s\tau)\,]\,F(z) \tag{13}$$

where, $P(z, s\tau)$, and $Q(z, s\tau)$ are

$$P(z,\ s\tau) = \sum_{i=0}^{p} R_i\ (s\tau)\ z^i\ , \tag{14}$$

and

$$Q(z,\ s\tau)=\sum_{j=0}^{l} T_j(s\tau)\, z^j \tag{15}$$

respectively. $P(z,s\tau)/Q(z,s\tau)$ in Eqs. (13) ∿ (15) obtained by using the approximation function $F(s\tau)$ correspond to the theoretical integration operator $H(z,s\tau)$ in Eqs. (8) and (9), and in this case,

$$P(z,\ s\tau)=0 \tag{16}$$

is called the characteristic equation. Typical existing numerical integration methods are listed in Table 1 in the form of Eq. (16). In order to evaluate the methods based on the criterion described in Section 2.1, the characteristic root in Eq. (16) which may be reduced to $z=F(s\tau)$, is considered.

$F(s\tau)$ is written as

$$z=F(i\omega\tau)=|F(i\omega\tau)|\angle F(i\omega\tau) \tag{17}$$

by the same way as Eq. (11) when $s=i\omega\tau$. $|F(i\omega\tau)|$ and $\angle F(i\omega\tau)$ are called gain and phase, and are put

$$|F(i\omega_0\tau)|=d\quad,\ \angle F(i\omega_0\tau)=\bar{\omega}_0\tau\ . \tag{18}$$

Corresponding to the nature of the function, $F(i\omega\tau)$ may have various gain and phase characteristics shown in Figs. 2(a) and 2(b).

Now, let us consider numerically integrating an undamped vibratory system having a natural frequency ω_0 every time mesh τ. For example, if we use an integration method having (G-c) and (P-c) properties in Figs. 2, the root of a state transition operator $F(i\omega_0\tau)$ is regarded as the root in z-plane shown in Fig. 3(b). Once more inverse mapping from a root in z-plane into a root in $s\tau$-plane comes to the pole distribution shown in Fig. 3(c). Accordingly, it can be seen that if we use the method described above, the solution $i\omega_0\tau$ (in Fig. 3(a)) on the imaginary axis of $s\tau$-plane consists with the solution $\sigma\tau+i\bar{\omega}_0\tau$ in $s\tau$-plane solved by the exact method. In the example herein, the real part and the imaginary part of the solution

$$\sigma\tau=\ln|F(i\omega_0\tau)|<0 \tag{19}$$

$$\bar{\omega}_0\tau=\angle F(i\omega_0\tau)<\omega_0\tau \tag{20}$$

Table 1. Characteristic equations of various integration operators and Padé approximation functions

	Integration Method and Approx. Func.	Characteristic equation
(a)	Adams Bashforth 2nd	$Z^2-(1+3S\tau/2)Z+S\tau/2=0$
	Adams Bashforth 3rd	$Z^3-(1+23S\tau/12)Z^2+4S\tau/3\cdot Z-5S\tau/12=0$
	Adams Moulton 3rd	$(1-\frac{5}{12}S\tau)Z^2-(1+8S\tau/12)Z+S\tau/12=0$
	Adams Bashforth Adams Moulton 2nd	$Z^2-(1+S\tau+3S^2\tau^2/4)Z+S^2\tau^2/4=0$
	Milne	$Z^4-(4S\tau/3+8S^2\tau^2/9)Z^3-(1+S\tau/3-4S^2\tau^2/9)Z^2$ $-8S^2\tau^2/9Z-S\tau/3=0$
	Milne Hammig modified	$8Z^4-(9+6S\tau+8S^2\tau^2)Z^3+(3S\tau+4S^2\tau^2)Z^2$ $-(8S^2\tau^2-1)Z-3S\tau=0$
	Stiffly stable 2nd	$(3-2S\tau)Z^2-4Z+1=0$
	Stiffly stable 3rd	$(11-6S\tau)Z^3-18Z^2+9Z-2=0$
	Midpoint trapezoidal	$Z^2-(1+S\tau/2+S^2\tau^2)Z-S\tau/2=0$
(b)	Houbolt	$(1+11\zeta\omega_n\tau/6+\omega_n^2\tau^2/2)Z^3-(5/2+3\zeta\omega_n\tau)Z^2$ $+(2+3\zeta\omega_n\tau/2)Z-(1/2+\zeta\omega_n\tau/3)=0$
	Newmark-β	$(1+\zeta\omega_n\tau+\beta\omega_n^2\tau^2)Z^2-2\{1+(\beta-\frac{1}{2})\omega_n^2\tau^2\}Z$ $+(1-\zeta\omega_n\tau+\beta\omega_n^2\tau^2)=0$
	Wilson-θ	$C_1Z^3+C_2Z^2+C_3Z+C_4=0$, $C_1=\theta+\theta^2\omega\tau\zeta+\theta^3\omega^2\tau^2/6$ $C_2=(1-3\theta)+(1+2\theta-3\theta^2)\omega\tau\zeta+(1+3\theta+3\theta^2-3\theta^3)\omega^2\tau^2/6$ $C_3=(3\theta-2)+(3\theta^2-4\theta)\omega\tau\zeta+(3\theta^3-6\theta^2+4)\omega^2\tau^2/6$ $C_4=(1-\theta)-(\theta^2-2\theta+1)\omega\tau\zeta-(\theta^3-3\theta^2+3\theta-1)\omega^2\tau^2/6$
(c)	Euler (Padé high pass type)	$Z-(1+S\tau)=0$
	Backward Euler (Padé low pass type)	$(1-S\tau)Z-1=0$
	Runge Kutta 3rd (Padé high pass type)	$Z-(1+S\tau+S^2\tau^2/2+S^3\tau^3/6)=0$
	Runge Kutta 4th (Padé high pass type)	$Z-(1+S\tau+S^2\tau^2/2+S^3\tau^3/6+S^4\tau^4/24)=0$
(d)	Diagonal Padé P_{11}	$(1-S\tau/2)Z-(1+S\tau/2)=0$
	Diagonal Padé P_{22}	$(1-S\tau/2+S^2\tau^2/12)Z-(1+S\tau/2+S^2\tau^2/12)=0$
	Diagonal Padé P_{33}	$(1-S\tau/2+S^2\tau^2/10-S^3\tau^3/120)Z$ $-(1+S\tau/2+S^2\tau^2/10+S^3\tau^3/120)=0$

Note (a) Integration operators for general use
(b) Integration operators for 2nd order ordinary differential equation, and $\zeta\tau, \omega_n\tau$ disignate $S\tau=-\zeta\omega_n\tau\pm i(1-\zeta^2\omega_n^2)^{1/2}\tau$,
(c) These are not only the operators for general use but also the families of Padé approximations to exponential function
(d) Diagonal Padé approximations

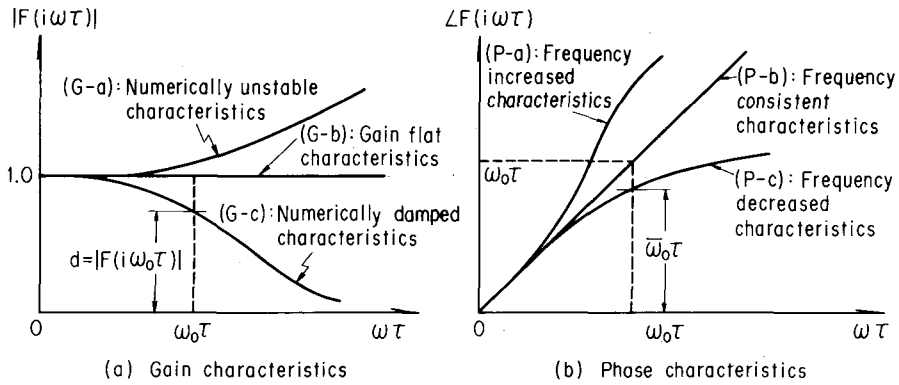


Fig. 2. Characteristics of numerical integration operators $F(s\tau)$

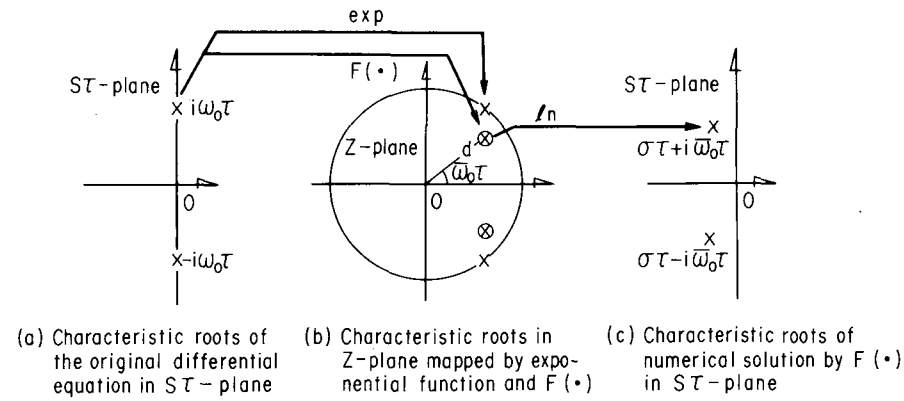


Fig. 3. Relationship between characteristic roots given by the theoritical solution and the numerical solution

are obtained and this solution is recognized to be solved as a damped lower frequency solution compared with the exact one. Similarly, all of the curves in Figs. 2 can be characterized to any one of ① ∿ ⑥. The characteristics of an integration operator can be classified to an arbitrary combination of gain (① ∿ ③) and phase characteristics (④ ∿ ⑥).

① G-a ; $\sigma > o$: Numerically unstable characteristics

② G-b ; $\sigma = o$: Gain flat characteristics

③ G-c ; $\sigma < o$: Numerically damped characteristics

④ P-a ; $\bar{\omega}_0 > \omega_0$: Frequency increased characteristics

⑤ P-b ; $\bar{\omega}_0 = \omega_0$: Frequency consistent characteristics

⑥ P-c ; $\bar{\omega}_0 < \omega_0$: Frequency decreased characteristics

2.3 Evaluation of Numerical Integration Method

Several typical integration methods were chosen from Table 1, and then evaluated by the method described in section 2.2. At the same time, diagonal Padé approximation functions to exponential function listed in the last of Table 1 were evaluated by the same method. Gain and phase characteristics are shown in Figs. 4 and 5. Characteristics of integration operators for general use of ordinary differential equations are shown in Fig. 4 and those of integration operators for second order ordinary differential equations are shown in Fig. 5. The characteristics of Padé's approximation functions are also shown in Fig. 5. Here, we are worth

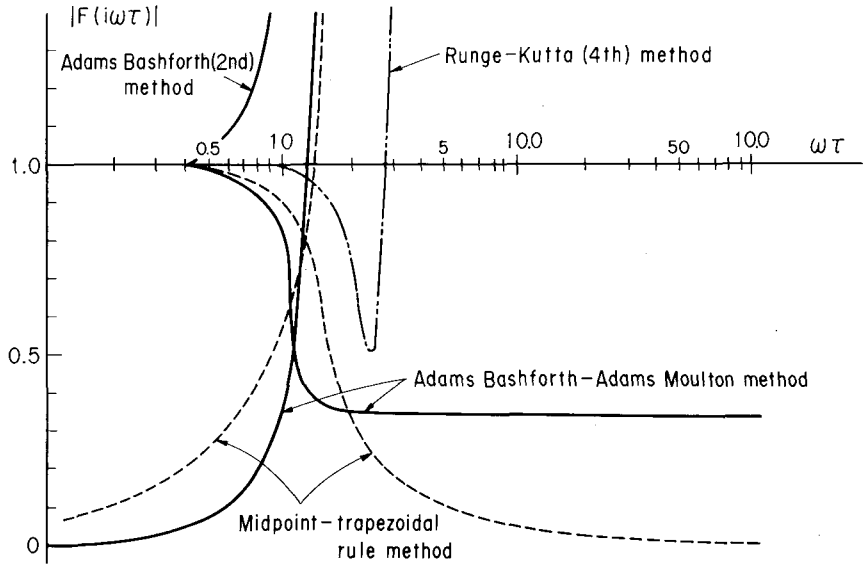


Fig. 4(a) Gain characteristics of integration operators for general use

paying attention to that Padé's approximation functions are considerably superior from the point of view of the integration operator evaluation.

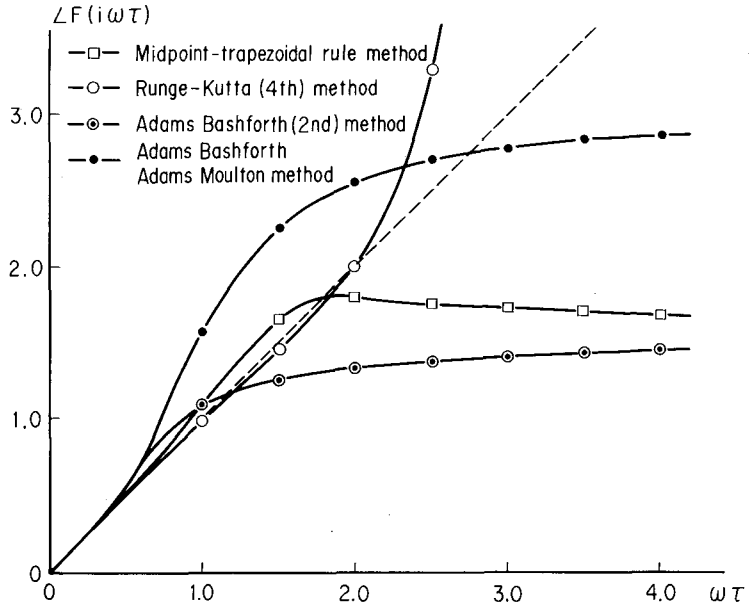


Fig. 4(b) Phase characteristics of integration operators for general use

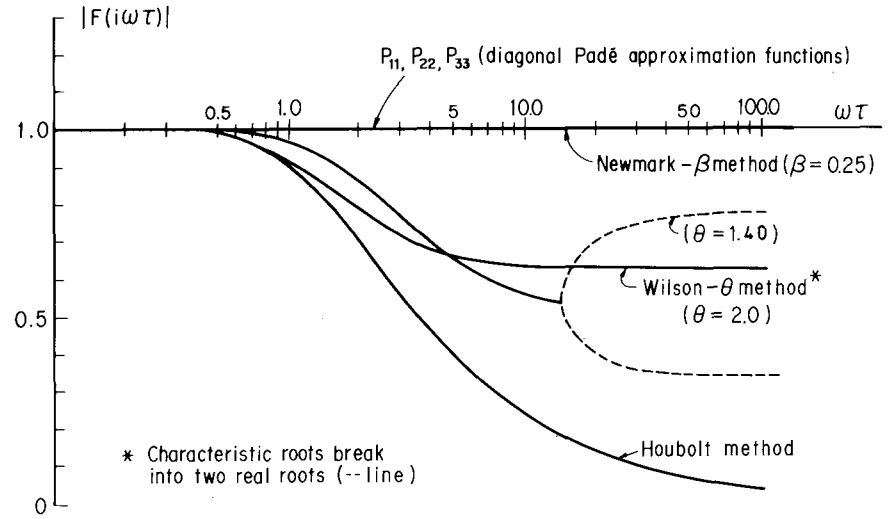


Fig. 5(a) Gain characteristics of integration operators for 2nd order ordinary differential equation and diagonal Padé approximation functions

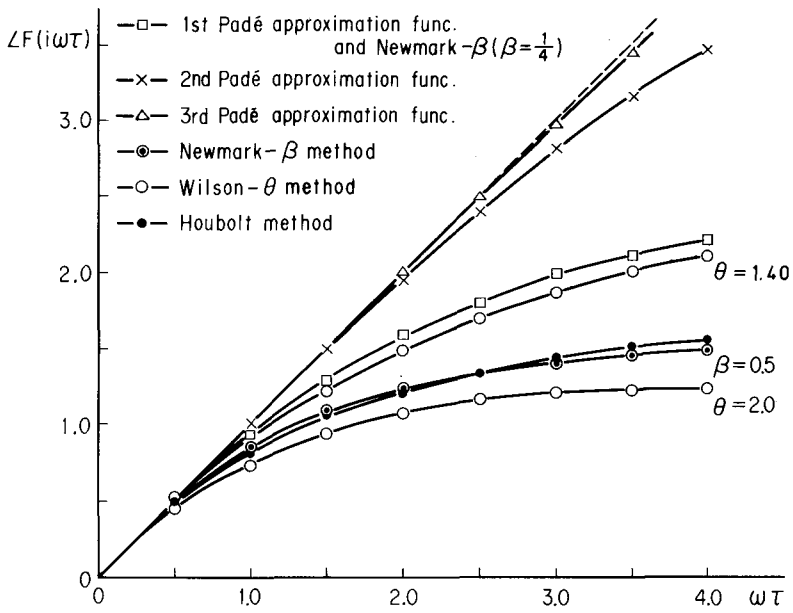


Fig. 5(b) Phase characteristics of integration operators for 2nd order ordinary differential equation and diagonal Padé approximation functions

3. Proposal of Direct Numerical Integration Methods for Large Scale Ordinary Differential Equations

In this chapter, new numerical integration methods for solving large scale simultaneous ordinary matrix differential equations which arise in dynamic analysis of structures and system simulations are discussed.

3.1 Necessary Conditions and Integration Operators for Numerical Integration Methods

3.1.1 Necessary Conditions for Numerical Integration Methods

Necessary conditions required in direct numerical integrations by an electronic digital computer are summarized as

(1) Fundamental characteristics (precision and stability) of the numerical integration method can be systematically evaluated,

(2) Numerical stability is guaranteed,

(3) Numerical precision is high,

(4) In computation, small amount of treatments is required and sparsity and bandness of a matrix can be effectively made use

of,

(5) Small memory (store) capacity is required and internal memories and external memories can be easily treated by simple routines,

from a view point of design specifications of an integration method for large scale ordinary differential equations.

The items (1) ∿ (4) and (4) ∿ (5) correspond to the design specifications in the case of making integration operator and integration algorithm, respectively.

3.1.2 Integration Operators Suitable for the Numerical Computation of Large Scale Ordinary Differential Equations

Integration operators suitable for the numerical computation of large scale ordinary differential equations are considered on the basis of the results obtained in sections 2.3 and 3.1.1. The most suitable function describing the state transition operator is the family of diagonal Padé approximation functions $\mathbf{P}_{pp}$ with which we concerned in chapter 2. That is the diagonal Padé approximation function has the following excellent properties; (1) Precision of the approximation function $\mathbf{P}_{pp}$ increases regularly with the approximation order p and precision and stability of $\mathbf{P}_{pp}$ as an integration operator can be simply and systematically evaluated, (2) The function $\mathbf{P}_{pp}$ as a state transition operator is numerically stable, (3) Precision of $\mathbf{P}_{11}$ is as well as that of Newmark-β method and precision of $\mathbf{P}_{22}$ is much higher than that of $\mathbf{P}_{11}$. Furthermore, if we consider the stage when integration algorithms are made, the following properties are added to the items described above; (4) Amount of treatments in computation is small, (5) Memory capacity required is also small.

From the above considerations, the studies are limited to the numerical integration method based on the diagonal Padé approximation function to the state transition matrix $e^{\mathbf{A}\tau}$. An integration operator based on the diagonal Padé approximation function is designed, made, and evaluated.

3.2 Basic Formulas of Numerical Integration Method

3.2.1 Basic Formulas for First Order Ordinary Differential Equations

Basic formulas for first order ordinary differential equations are described as Eqs. (1), (3), and (4) in chapter 2.

When non-linear systems are dealt with, these equations are assumed to be approximated to piece-wise linear systems.

(a) Approximation of Forcing Vector

Equations which seem to be particularly important in practice are listed in Table 2 setting l=0 and 1 in Eq. (4). The forcing vectors for l =0 and 1 correspond to step-wise and ramp-wise approximations in time domain, respectively.

Table 2. Difference equations derived from approximation of forcing vector

ℓ	Difference equation	Forcing vector approximation
0	$\mathbf{y}_{n+1}=e^{\mathbf{A}\tau}\mathbf{y}_n+(e^{\mathbf{A}\tau}-\mathbf{I})\mathbf{A}^{-1}\mathbf{B}\mathbf{f}_n$	$\mathbf{f}_n(\eta)=\mathbf{f}_n^{(0)}\equiv\mathbf{f}_n$
1	$\mathbf{y}_{n+1}=e^{\mathbf{A}\tau}\mathbf{y}_n+e^{\mathbf{A}\tau}\mathbf{A}^{-1}\mathbf{B}\mathbf{f}_n-\mathbf{A}^{-1}\mathbf{B}\mathbf{f}_{n+1}$ $+(e^{\mathbf{A}\tau}-\mathbf{I})\mathbf{A}^{-2}\mathbf{B}(\mathbf{f}_{n+1}-\mathbf{f}_n)/\tau$	$\mathbf{f}_n(\eta)=\mathbf{f}_n+\eta\mathbf{f}_n^{(1)}$ $\mathbf{f}_n^{(1)}\equiv(\mathbf{f}_{n+1}-\mathbf{f}_n)/\tau$

(b) Approximation of State Transition Matrix

The pth diagonal Padé approximation function (expansion formula with real coefficients),

$$e^{\mathbf{A}\tau}\cong\mathbf{P}_{pp}=\mathbf{D}_{R,p}^{-1}\cdot\mathbf{N}_{R,p} \tag{21}$$

$$\mathbf{D}_{R,p}=\sum_{K=0}^{p}\frac{p!\,(2p-k)!}{(2p)!\,(p-k)!\,k!}(-\mathbf{A}\tau)^k \tag{22}$$

$$\mathbf{N}_{R,p}(\mathbf{A}\tau)=\mathbf{D}_{R,p}(-\mathbf{A}\tau) \tag{23}$$

is used as an approximation to the state transition matrix $e^{\mathbf{A}\tau}$. Equations for p= 1∿4 of Eqs. (21) ∿ (23) are listed in Table 3.

Next, a representation being equivalent to Eq. (21) is considered. The $\mathbf{P}_{pp}$ in Eq. (21) can be alternatively represented as

$$e^{\mathbf{A}\tau}\cong\mathbf{P}_{pp}=\mathbf{D}_{C,p}^{-1}\cdot\mathbf{N}_{C,p} \tag{24}$$

$$\mathbf{D}_{C,p}=\prod_{k=1}^{p}(\mathbf{I}-\mathbf{A}\tau/c_k) \tag{25}$$

$$\mathbf{N}_{C,p}(\mathbf{A}\tau)=\mathbf{D}_{C,p}(-\mathbf{A}\tau) \tag{26}$$

using the complex coefficients (expansion formula with complex coefficients). Complex coefficients c_k for $p=1\sim4$ of Eqs. (24)$\sim$(26) are listed in Table 4. The values c_k correspond to the roots of Eq. (25).

Table 3. Approximation formulas of the state transition matrix e^{AT} (expansion with real coefficients)

p	$D_{R,p}$, $N_{R,p}$ *	P_{pp} **
1	$I \mp \frac{A\tau}{2}$	$I + A\tau + \cdots + \left[\frac{(A\tau)^3}{4}\right] + \cdots$
2	$I \mp \frac{A\tau}{2} + \frac{(A\tau)^2}{12}$	$I + A\tau + \cdots + \left[\frac{(A\tau)^5}{144}\right] + \cdots$
3	$I \mp \frac{A\tau}{2} + \frac{(A\tau)^2}{10} \mp \frac{(A\tau)^3}{120}$	$I + A\tau + \cdots + \left[\frac{(A\tau)^7}{4800}\right] + \cdots$
4	$I \mp \frac{A\tau}{2} + \frac{3(A\tau)^2}{28} \mp \frac{(A\tau)^3}{84} + \frac{(A\tau)^4}{1680}$	$I + A\tau + \cdots + \left[\frac{1.969\times10^{-5}}{1.69344}(A\tau)^9\right] +$
Note	* For $N_{R,p}$, the signs of lower part of each row are selected ** pth Taylor expansion coefficient of $e^{A\tau}$ is $(A\tau)^p / p!$	

Table 4. Roots of diagonal Padé approximation functions

p	C_K		
	k	real·part	imag·part
1	1	2.0	0.0
2	1	3.0	1.732050
	2	3.0	-1.732050
3	1	3.677814	3.508761
	2	3.677814	-3.508761
	3	4.644371	0.0
4	1	5.792421	1.734467
	2	5.792421	-1.734467
	3	4.207578	5.314835
	4	4.207578	-5.314835

(c) Difference Formulas using l th Forcing Vector Approximation and p th State Transition Matrix Approximation

First of all, equations by using the expansion formula with real coefficients in the p th diagonal Padé approximation function to the state transition matrix ${}_e\mathbf{A}\tau$ are considered. Substituting Eq. (21) into (4).

$$\mathbf{D}_{R,p}\,\mathbf{y}_{n+1}=\mathbf{N}_{R,p}\,\mathbf{y}_n+\sum_{i=0}^{l}(\mathbf{A}_1-\mathbf{D}_{R,p}\,\mathbf{A}_2)\,\mathbf{B}\,\mathbf{f}_n^{(i)} \tag{27}$$

$$\left.\begin{aligned}\mathbf{A}_1&=\sum_{1=1,3,5,\cdots}\{2\cdot p!\,(2p-m)!/((2p)!(p-m)!m!)\}\tau^m\mathbf{A}^{m-(i+1)}\\ \mathbf{A}_2&=\sum_{i=0}^{i-1}\frac{1}{(i-r)!}\,\tau^{i-r}\mathbf{A}^{-(r+1)}\end{aligned}\right\} \tag{28}$$

are obtained. Difference equations for $l=0,\ 1$; $p=1\sim4$ of Eq. (27) are listed in Table 5.

Table 5. Difference equations for single order ordinary differential equation by using diagonal Padé approximation functions

p \ l*	1
1	$(\mathrm{I}-\frac{\mathbf{A}\tau}{2})\mathbf{y}_{n+1}=(\mathrm{I}+\frac{\mathbf{A}\tau}{2})\mathbf{y}_n+\frac{\tau}{2}\mathbf{B}\,(\mathbf{f}_{n+1}+\mathbf{f}_n)$
2	$(\mathrm{I}-\frac{\mathbf{A}\tau}{2}+\frac{(\mathbf{A}\tau)^2}{12})\mathbf{y}_{n+1}=(\mathrm{I}+\frac{\mathbf{A}\tau}{2}+\frac{(\mathbf{A}\tau)^2}{12})\mathbf{y}_n+\frac{\tau}{2}\mathbf{B}(\mathbf{f}_{n+1}+\mathbf{f}_n)-\frac{\mathbf{A}\tau^2}{12}\mathbf{B}\,(\mathbf{f}_{n+1}-\mathbf{f}_n)$
3	$(\mathrm{I}-\frac{\mathbf{A}\tau}{2}+\frac{(\mathbf{A}\tau)^2}{10}-\frac{(\mathbf{A}\tau)^3}{120})\mathbf{y}_{n+1}=(\mathrm{I}+\frac{\mathbf{A}\tau}{2}+\frac{(\mathbf{A}\tau)^2}{10}+\frac{(\mathbf{A}\tau)^3}{120})\mathbf{y}_n+\frac{\tau}{2}\mathbf{B}(\mathbf{f}_{n+1}+\mathbf{f}_n)-\frac{\mathbf{A}\tau^2}{12}\mathbf{B}(\mathbf{f}_{n+1}-\mathbf{f}_n)+\frac{\mathbf{A}^2\tau^3}{120}\mathbf{B}(\mathbf{f}_{n+1}+\mathbf{f}_n)$
4	$(\mathrm{I}-\frac{\mathbf{A}\tau}{2}+\frac{3(\mathbf{A}\tau)^2}{28}-\frac{(\mathbf{A}\tau)^3}{84}+\frac{(\mathbf{A}\tau)^4}{1680})\mathbf{y}_{n+1}=(\mathrm{I}+\frac{\mathbf{A}\tau}{2}+\frac{3(\mathbf{A}\tau)^2}{28}+\frac{(\mathbf{A}\tau)^3}{84}+\frac{(\mathbf{A}\tau)^4}{1680})\mathbf{y}_n+\frac{\tau}{2}\mathbf{B}(\mathbf{f}_{n+1}+\mathbf{f}_n)-\frac{\mathbf{A}\tau^2}{12}\mathbf{B}(\mathbf{f}_{n+1}-\mathbf{f}_n)+\frac{\mathbf{A}^2\tau^3}{84}\mathbf{B}(\mathbf{f}_{n+1}+\mathbf{f}_n)-\frac{\mathbf{A}^3\tau^4}{1680}\mathbf{B}(\mathbf{f}_{n+1}-\mathbf{f}_n)$
Note	* In case of $l=0$, $\mathbf{f}_{n+1}$ is replaced by $\mathbf{f}_n$ (i. e, $\mathbf{f}_{n+1}\rightarrow\mathbf{f}_n$)

Next, equations by using the expansion formula with complex coefficients in the pth diagonal Padé approximation function to the state transition matrix $e^{\mathbf{A}\tau}$ are considered. Substituting Eq. (24) into (4), one gets

$$\mathbf{D}_{C,p}\ \mathbf{y}_{n+1} = \mathbf{N}_{C,p}\ \mathbf{y}_n + \sum_{i=0}^{l} (\mathbf{A}_1 - \mathbf{D}_{C,p}\ \mathbf{A}_2)\ \mathbf{B}\ \mathbf{f}_n^{(i)} \quad (29)$$

Then, substitution of a discrete representation

$$\mathbf{A}\ \mathbf{y}_n^{(i)} = \mathbf{y}_n^{(i+1)} - \mathbf{B}\ \mathbf{f}_n^{(i)} \quad (30)$$

of the derivatives of Eq. (1) into Eq. (29) gives the equations listed in Table 6 for $l=0, 1$; $p=2$. As for the equation for $p=1$, it is consistent with the equation listed in Table 5.

Table 6. Difference equations for single order ordinary differential equation by using diagonal Padé approximation functions (expansion with complex coefficients)

p \ l	0	1
2	$(I-\frac{\tau}{c_1}\mathbf{A})\mathbf{w}_{n+1}=\tau\mathbf{A}\mathbf{y}_n+\tau\mathbf{B}\mathbf{f}_n$	$(I-\frac{\tau}{c_1}\mathbf{A})\mathbf{w}_{n+1}=\tau\dot{\mathbf{y}}_n+\frac{\tau}{c_1}\mathbf{B}(\mathbf{f}_{n+1}-\mathbf{f}_n)$
	$\tau\mathbf{A}\mathbf{y}_{n+1}=\tau\mathbf{A}\mathbf{y}_n-4\sqrt{3}\,\mathrm{Im}(\mathbf{w}_{n+1})$	$\tau\dot{\mathbf{y}}_{n+1}=\tau\dot{\mathbf{y}}_n-4\sqrt{3}\,\mathrm{Im}(\mathbf{w}_{n+1})$
	$\mathbf{y}_{n+1}=\mathbf{y}_n+\mathrm{Re}(\mathbf{w}_{n+1})-\sqrt{3}\,\mathrm{Im}(\mathbf{w}_{n+1})$	$\mathbf{y}_{n+1}=\mathbf{y}_n+\mathrm{Re}(\mathbf{w}_{n+1})-\sqrt{3}\,\mathrm{Im}(\mathbf{w}_{n+1})$
	$\mathbf{w}_{n+1}\equiv(\mathbf{y}_{n+1}-\mathbf{y}_n)-\frac{\tau}{c_2}\mathbf{A}(\mathbf{y}_{n+1}-\mathbf{y}_n)$	$\mathbf{w}_{n+1}\equiv(\mathbf{y}_{n+1}-\mathbf{y}_n)-\frac{\tau}{c_2}(\dot{\mathbf{y}}_{n+1}-\dot{\mathbf{y}}_n)$
	$c_1 = 3 + i\sqrt{3}$	$c_2 = 3 - i\sqrt{3}$

3.2.2 Basic Formulas for Second Order Ordinary Differential Equations

Let us consider the equation

$$\mathbf{M}\ddot{\mathbf{x}} + \mathbf{C}\dot{\mathbf{x}} + \mathbf{K}\mathbf{x} = \mathbf{f} \quad (31)$$

arising in structural dynamics. In the case of dealing with a non-linear system, the equation is assumed to be approximated to the piece-wise linear systems. In order to represent Eq. (31) in the form of Eq. (1), $\mathbf{y}$, $\mathbf{A}$ and $\mathbf{B}$ must be written as

$$\mathbf{y}=\begin{bmatrix}\mathbf{x}\\ \dot{\mathbf{x}}\end{bmatrix},\quad \mathbf{A}=\begin{bmatrix}\mathbf{0} & \mathbf{I}\\ -\mathbf{M}^{-1}\mathbf{K} & -\mathbf{M}^{-1}\mathbf{C}\end{bmatrix}\qquad \mathbf{B}=\begin{bmatrix}\mathbf{0}\\ \mathbf{M}^{-1}\end{bmatrix} \tag{32}$$

in terms of $\mathbf{M}$, $\mathbf{C}$ and $\mathbf{K}$. Here, denoting a discrete variable at time $t=n\tau$ as

$$\mathbf{y}_n=\begin{bmatrix}\mathbf{x}_n\\ \dot{\mathbf{x}}_n\end{bmatrix}=\begin{bmatrix}\mathbf{x}\\ \dot{\mathbf{x}}\end{bmatrix}_n\quad , \tag{33}$$

a difference equation is obtained using the variable $\mathbf{y}_n$.

Firstly, when the expansion formula with real coefficients in the pth diagonal Padé approximation function is used to the state transition matrix $e^{\mathbf{A}\tau}$, desired formulas can be obtained by substituting Eqs. (32) and (33) into (27). Doing this, the formulas for $l=0, 1$; $p=1, 2$ are obtained and listed in Table 7.

Table 7. Difference equations for single order ordinary differential equation by using diagonal Padé approximation functions (expansion with complex coefficients)

p \ l	0	1
1	PR-01; $\mathbf{R}\dot{\mathbf{x}}_{n+1}=\mathbf{T}\dot{\mathbf{x}}_n-2\mathbf{K}\mathbf{x}_n+2\mathbf{f}_n$ $\mathbf{x}_{n+1}=\mathbf{x}_n+\frac{\tau}{2}(\dot{\mathbf{x}}_{n+1}+\dot{\mathbf{x}}_n)$ $\ddot{\mathbf{x}}_{n+1}=-\ddot{\mathbf{x}}_n+\frac{2}{\tau}(\dot{\mathbf{x}}_{n+1}-\dot{\mathbf{x}}_n)+\mathbf{M}^{-1}(\mathbf{f}_{n+1}-\mathbf{f}_n)$	PR-11; $\mathbf{R}\dot{\mathbf{x}}_{n+1}=\mathbf{T}\dot{\mathbf{x}}_n-2\mathbf{K}\mathbf{x}_n+(\mathbf{f}_{n+1}+\mathbf{f}_n)$ $\mathbf{x}_{n+1}=\mathbf{x}_n+\frac{\tau}{2}(\dot{\mathbf{x}}_{n+1}+\dot{\mathbf{x}}_n)$ $\ddot{\mathbf{x}}_{n+1}=-\ddot{\mathbf{x}}_n+\frac{2}{\tau}(\dot{\mathbf{x}}_{n+1}-\dot{\mathbf{x}}_n)$
	$\mathbf{R}=\frac{2}{\tau}\mathbf{M}+\mathbf{C}+\frac{\tau}{2}\mathbf{K}$, $\mathbf{T}=\frac{2}{\tau}\mathbf{M}-\mathbf{C}-\frac{\tau}{2}\mathbf{K}$	
2	PR-02; $\begin{pmatrix}\mathbf{R} & \mathbf{S}\\ \mathbf{S} & \mathbf{T}\end{pmatrix}\begin{pmatrix}\mathbf{x}\\ \dot{\mathbf{x}}\end{pmatrix}_{n+1}=\begin{pmatrix}\mathbf{U} & \mathbf{S}\\ \mathbf{S} & \mathbf{V}\end{pmatrix}\begin{pmatrix}\mathbf{x}\\ \dot{\mathbf{x}}\end{pmatrix}_n+\begin{pmatrix}\tau\mathbf{f}_n\\ \mathbf{0}\end{pmatrix}$ $\ddot{\mathbf{x}}_{n+1}=\ddot{\mathbf{x}}_n+\frac{6}{\tau}(\dot{\mathbf{x}}_{n+1}+\dot{\mathbf{x}}_n)-\frac{12}{\tau^2}(\mathbf{x}_{n+1}-\mathbf{x}_n)+\mathbf{M}^{-1}(\mathbf{f}_{n+1}-\mathbf{f}_n)$	PR-12; $\begin{pmatrix}\mathbf{R} & \mathbf{S}\\ \mathbf{S} & \mathbf{T}\end{pmatrix}\begin{pmatrix}\mathbf{x}\\ \dot{\mathbf{x}}\end{pmatrix}_{n+1}=\begin{pmatrix}\mathbf{U} & \mathbf{S}\\ \mathbf{S} & \mathbf{V}\end{pmatrix}\begin{pmatrix}\mathbf{x}\\ \dot{\mathbf{x}}\end{pmatrix}_n+\begin{pmatrix}\frac{\tau}{2}(\mathbf{f}_{n+1}+\mathbf{f}_n)\\ -\frac{\tau^2}{12}(\mathbf{f}_{n+1}-\mathbf{f}_n)\end{pmatrix}$ $\ddot{\mathbf{x}}_{n+1}=\ddot{\mathbf{x}}_n+\frac{6}{\tau}(\dot{\mathbf{x}}_{n+1}+\dot{\mathbf{x}}_n)-\frac{12}{\tau^2}(\mathbf{x}_{n+1}-\mathbf{x}_n)$
	$\mathbf{R}=\mathbf{C}+\frac{\tau}{2}\mathbf{K}$, $\mathbf{S}=\mathbf{M}-\frac{\tau^2}{12}\mathbf{K}$, $\mathbf{T}=-(\frac{\tau}{2}\mathbf{M}+\frac{\tau^2}{12}\mathbf{C})$ $\mathbf{U}=\mathbf{C}-\frac{\tau}{2}\mathbf{K}$, $\mathbf{V}=\frac{\tau}{2}\mathbf{M}-\frac{\tau^2}{12}\mathbf{C}$	

Secondly, let us obtain the difference equation using the expansion formula with complex coefficients as the pth diagonal Padé approximation function to the state transition matrix $e^{\mathbf{A}\tau}$. Desired formulas for $l = 0$, $l = 1$; $p = 2$ (PC-12 method) are obtained as Table 8.

Table 8. Difference equations for 2nd order ordinary differential equation by using diagonal Padé approximation functions (expansion with complex coefficients)

p \ l	0	1
2	PC-02 ; $\mathbf{R}\mathbf{w}_{n+1} = -\tau\mathbf{K}\mathbf{x}_n + C_1\mathbf{M}\dot{\mathbf{x}}_n + \tau\mathbf{f}_n$ $\mathbf{x}_{n+1} = \mathbf{x}_n + R_e(\mathbf{w}_{n+1}) - \sqrt{3}\, I_m(\mathbf{w}_{n+1})$ $\dot{\mathbf{x}}_{n+1} = \dot{\mathbf{x}}_n - \frac{4\sqrt{3}}{\tau} I_m(\mathbf{w}_{n+1})$ $\ddot{\mathbf{x}}_{n+1} = \ddot{\mathbf{x}}_n + \frac{6}{\tau}(\dot{\mathbf{x}}_{n+1} + \dot{\mathbf{x}}_n) - \frac{12}{\tau^2}(\mathbf{x}_{n+1} - \mathbf{x}_n) + \mathbf{M}^{-1}(\mathbf{f}_{n+1} - \mathbf{f}_n)$	PC-12 ; $\mathbf{R}\mathbf{w}_{n+1} = -\tau\mathbf{K}\mathbf{x}_n + C_1\mathbf{M}\dot{\mathbf{x}}_n + \frac{\tau}{2}(\mathbf{f}_{n+1} + \mathbf{f}_n) - \frac{C_1\tau}{12}(\mathbf{f}_{n+1} - \mathbf{f}_n)$ $\mathbf{x}_{n+1} = \mathbf{x}_n + R_e(\mathbf{w}_{n+1}) - \sqrt{3}\, I_m(\mathbf{w}_{n+1})$ $\dot{\mathbf{x}}_{n+1} = \dot{\mathbf{x}}_n - \frac{4\sqrt{3}}{\tau} I_m(\mathbf{w}_{n+1})$ $\ddot{\mathbf{x}}_{n+1} = \ddot{\mathbf{x}}_n + \frac{6}{\tau}(\dot{\mathbf{x}}_{n+1} + \dot{\mathbf{x}}_n) - \frac{12}{\tau^2}(\mathbf{x}_{n+1} - \mathbf{x}_n)$
	$\mathbf{w}_{n+1} \equiv (\mathbf{x}_{n+1} - \mathbf{x}_n) - \frac{C_1\tau}{12}(\dot{\mathbf{x}}_{n+1} - \dot{\mathbf{x}}_n)$, $\mathbf{R} = \frac{C_1}{\tau}\mathbf{M} + \mathbf{C} + \frac{\tau}{C_1}\mathbf{K}$ $C_1 = 3 + i\sqrt{3}$	

Formulas for higher order of p (for example $p = 3$) will also be arranged, but descriptions are omitted herein.

3.3 Algorithms and Their Performance of Proposed Numerical Integration Methods

3.3.1 Algorithms of Numerical Integration Method

The algorithms which were made by the basic formulas obtained in section 3.2.2 are presented. The results are listed in Table 9. In order to analyze not only linear systems but also non-linear systems, the algorithms are given in the form of a piece-wise linearization.

Table 9. PC-12 algarithm of proposed direct numerical integration method

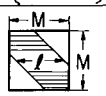
PC − 12 Algorithm
1) Computation of several coefficients and setting initial values
$a_1 = (3+i\sqrt{3})/\tau$, $a_2 = \tau/(3+i\sqrt{3})$, $b_1 = 6/\tau$, $b_2 = 12/\tau^2$ $b_3 = 4\sqrt{3}/\tau$, $b_4 = \tau/2$, $b_5 = (3+i\sqrt{3})\tau/12$, $c_1 = 3+i\sqrt{3}$, $n = 0$
2) Computation of the initial coefficient matrix $\mathbf{R}_0$
$\mathbf{R}_0 = a_1 \mathbf{M}_0 + \mathbf{C}_0 + a_2 \mathbf{K}_0$
3) Decomposition of the matrix $\mathbf{R}_0$ into L and R matrices for 4)-② (LR decomposition of $\mathbf{R}_0$)
4) Repetition for a computational time increment
① $\mathbf{y} = -\tau \mathbf{K}_n \mathbf{x}_n + c_1 \mathbf{M}_n \dot{\mathbf{x}}_n + b_4(\mathbf{f}_{n+1} + \mathbf{f}_n) - b_5(\mathbf{f}_{n+1} - \mathbf{f}_n)$ ② $\mathbf{R}_n \mathbf{w}_{n+1} = \mathbf{y} \rightarrow \mathbf{w}_{n+1}$ is obtained ②′ $\dot{\mathbf{x}}_{n+1} = \dot{\mathbf{x}}_n - b_3 I_m(\mathbf{w}_{n+1}) \rightarrow \dot{\mathbf{x}}_{n+1}$ is obtained ③ $\mathbf{x}_{n+1} = \mathbf{x}_n + R_e(\mathbf{w}_{n+1}) - 3 I_m(\mathbf{w}_{n+1}) \rightarrow \mathbf{x}_{n+1}$ is obtained ④ $\ddot{\mathbf{x}}_{n+1} = \ddot{\mathbf{x}}_n + b_1(\dot{\mathbf{x}}_{n+1} + \dot{\mathbf{x}}_n) - b_2(\mathbf{x}_{n+1} - \mathbf{x}_n) \rightarrow \ddot{\mathbf{x}}_{n+1}$ is obtained ⑤ Judgement of linearity of the system, if the system is linear, the flow must be jumped to ⑩, and if nonlinear, it jumped to ⑥ ⑥ Judgement of the variation of a coefficient matrix $\mathbf{R}$, if the elements vary, the flow must be jumped to ⑦, and if not, it jumped to ⑨ ⑦ Computation of the coefficient matrix $\mathbf{R}_{n+1}$ $\mathbf{R}_{n+1} = a_1 \mathbf{M}_{n+1} + \mathbf{C}_{n+1} + a_2 \mathbf{K}_{n+1}$ ⑧ Decomposition of the matrix $\mathbf{R}_{n+1}$ into L and R matrices for 4)-② (LR decomposition of $\mathbf{R}_{n+1}$). Jump to ⑩ ⑨ Replacement $\mathbf{R}_n$ by $\mathbf{R}_{n+1}$ because of the invariance of the matrix elements $\mathbf{R}_{n+1} = \mathbf{R}_n$ ⑩ Replacement n by n+1, then return ①
Note; $\mathbf{R}_n$, $\mathbf{y}$, $\mathbf{w}_{n+1}$ are complex vectors, $R_e(\ )$: real part $\mathbf{x}_{n+1}$, $\dot{\mathbf{x}}_{n+1}$, $\ddot{\mathbf{x}}_{n+1}$ are real vectors, $I_m(\ )$: imag. part

3.3.2 Performance of the Algorithms

Properties of the proposed integration methods and other typical integration methods are studied from the view point of performance of the algorithms. In table 10, memory capacity, amount of treatments in computation, and theoretical precision are listed

making performance of algorithms clear. Matrices considered are all assumed to be real banded. Almost same memory capacity is required in PR-11 (see Table 7), Newmark-β, and Wilson-θ methods, and Houbolt and PC-12 methods require about 1.3 times memory capacity of three methods described above. If the processing speed of a complex multiplication is assumed to be about half that of a real one, PR-11 is the fastest, and Newmark-β, Wilson-θ Houbolt, PC-12 methods follow in computational speed. PC-12 method is the best, PR-11 and Newmark-β methods are almost same and Wilson-θ and Houbolt methods follow in their precision. In synthetic performance, PC-12 method seems to be the most superior to other methods because of the extremely high precision in the method.

Table 10. Comparisons of characteristics of each integration method (for asymmetric matrix)

Method	Memory capacity	Amount of treatments *		Precision
		Multiplication	Addition	
PC − 12	$2a+b+11M$	$2a+b+9M$	$2a+b+12M$	$O[(s\tau)^5]$
PR − 11	$3a+6M$	$3a+2M$	$3a+10M$	$O[(s\tau)^3]$
Newmark−β	$3a+8M$	$3a+5M$	$3a+8M$	$O[(s\tau)^3]$
Wilson− θ	$3a+10M$	$3a+7M$	$3a+9M$	less equal $O[(s\tau)^3]$
Houbolt	$4a+7M$	$4a+8M$	$4a+12M$	less equal $O[(s\tau)^3]$
Note	ℓ ; Band width, M ; Matrix size, a ; for real, ** $a=b=M+(\ell-1)(M-\frac{\ell+1}{4})$, b ; for complex			

* This value indicates the one for a single step

** When the matrices are symmetric

$$a=b=M+(\ell-1)(M-\frac{\ell+1}{4})/2$$

4. Numerical Experiments and the Results

The aim of this chapter is to numerically confirm the fact that has been theoretically described in chapters 2 and 3. A computer program was made on the basis of the algorithm given in chapter 3. Furthermore, programs of the typical integration methods considered in chapter 2 were prepared. The programs numerically

computed the problems of a simple structure (a single mass-spring vibratory system) and rather complicated structures (multi mass-spring vibratory systems).

4.1 Numerical Experiments of a Single Mass-spring Vibratory System

In this section, the evaluation method of the integration operator described in chapter 2 will be confirmed by the computational results obtained by the programs of each integration method. A single mass-spring vibratory system shown in Fig. 6 is considered. The differential equation of the system is written as

$$\ddot{x} + \omega_0^2 \; x = f \tag{34}$$

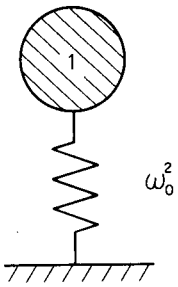


Fig. 6. Single undamped mass-spring vibratory system

Forcing function applying to the system is a unit step function. Inditial response of the system was computed by each integration method. Experimental condition for numerical computations is $\omega_0 \tau = 1.0$ ($\omega_0{}^2 = 39.473418$ (rad/s) ($f_0 = 1.0$ Hz), $\tau = 0.1591549$ s). Computational results are shown in Fig. 7.

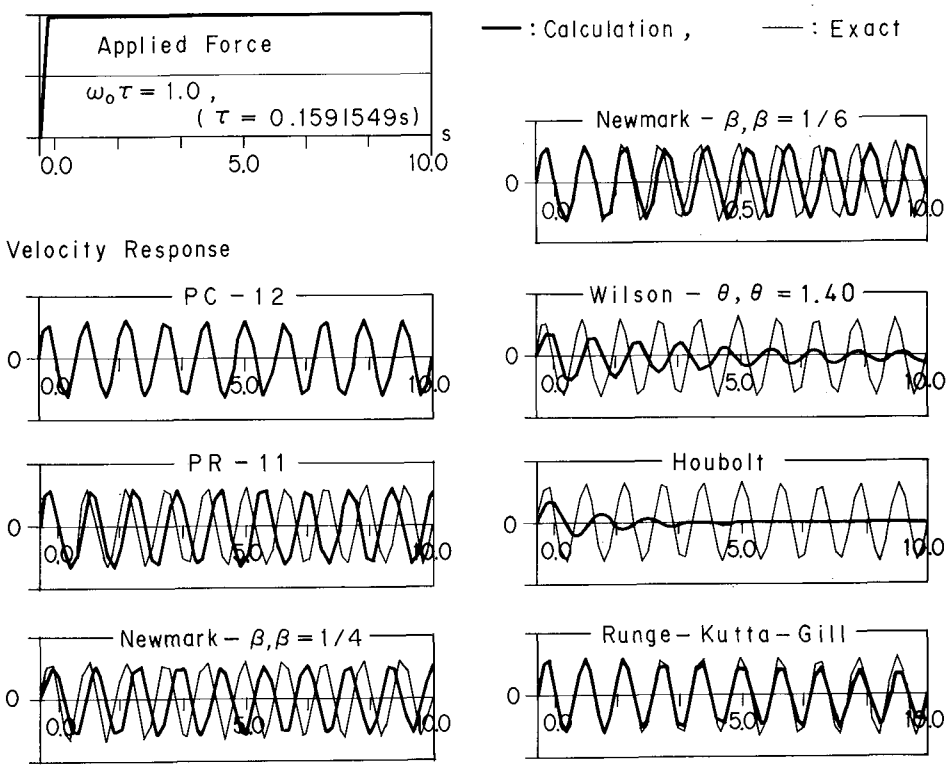


Fig. 7. Camputational results of a single undamped mass-spring vibratory system by using various numerical integration methods (in case of $\omega_0\tau$=1.0)

By the results obtained from the curves in Fig. 7, the characteristics of each integration method described in chapter 2 were numerically confirmed and consequently, the evaluating methods of numerical integration given in chapter 2 were proved to be appropriate.

4.2 Numerical Experiments of Multi Mass-spring Vibratory Systems

Z-shaped beam, shear beam, and T-shaped beam were discretized to multi mass-spring vibratory systems by means of the finite element method and were numerically computed by each integration method, and computational times required were compared with each

other. The results are listed in Table 11.

Table 11. Comparisons of computation time for each integration method used (Computation was done for 1,000 steps and step size was 0.01s)

Analysis model	shape	Z shaped beam	shear type	T shaped beam	note
	degree of freedom	60	30	24	
	band width	21	3	15	
Integration method	PC-12	2.15.72	22.06	40.31	
	PR-11	1.11.13	10.52	19.57	
	Newmark-β*	—	1.20.25	52.11	$\beta = \frac{1}{4}$
	Wilson-θ	2.10.44	27.79	26.91	$\theta = 1.40$
	Houbolt	3.38.25	55.89	37.12	
	RKG	—	1.14.59	—	

* Newmark-β method indicates generalized Newmark-β method developed by Chan. Computations were done by obtaining inverse matrix, so the comparisons are not fair, If the computation will be done by solving simultaneous equations, computation time is only needed almost equal to that of Wilson-θ method

IBM 370/158 K, min. sec. 1/100 sec, — ; diverge

From the discussions in sections 4.1 and 4.2, PC-12 method was proved to be the best one with respect to precision and PR-11 to be the most effective one to computational speed.

5. Conclusions

From this study, the authors obtained the following conclusions;

(1) It was proved that noting the distribution of the roots of characteristic equation of integration operator in $s\tau$-plane and in z-plane is effective as a method of systematically evaluating an integration operator. Considerations on the characteristic equations and characteristic roots of integration operator gave the evaluation results of operators and

they were summarized in figures and tables.

(2) The diagonal Padé approximation functions to exponential function were shown to be excellent as an integration operator by the result of evaluation of many integration operators.

(3) New direct numerical integration methods, PR-11 and PC-12, were proposed for large scale ordinary differential equations. The methods were found to be superior to Newmark-β method or Wilson-θ method.

(4) By the results of numerical computations, the characteristics of integration operator evaluated in chapter 2 were confirmed, and consequently the evaluation method proposed herein was proved to be reasonable. Furthermore, the numerical integration method, PC-12 proposed in chapter 3, was found to be the most suitable one judging from the synthetic performance with respect to memory capacity required, computational speed, and precision in the methods with which we concerned for large scale ordinary differential equations.

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