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STRUCTURE-PRESERVING ALGORITHMS FOR DYNAMICAL SYSTEMS*

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Abstract

We study structure-preserving algorithms to phase space volume for linear dynamical systems $\dot{y} = Ly$ for which arbitrarily high order explicit symmetric structure-preserving schemes,i.e. the numerical solutions generated by the schemes satisfy $\det(\frac{\partial y_1}{\partial y_0}) = e^{htrL}$, where trL is the trace of matrix L, can be constructed. For nonlinear dynamical systems $\dot{y} = f(y)$ Feng-Shang first-order volume-preserving scheme can be also constructed starting from modified θ - methods and is shown that the scheme is structure-preserving to phase space volume.

Key words: structure-preserving algorithm, phase space volume, source-free dynamical system.

1. Introduction

Consider the ODE_S

$$\frac{dy}{dt} = f(y),\ y \in \Re^n \tag{1.1}$$

with solutions $y(t)$ and Jacobian $B(t) = \frac{\partial y(t)}{\partial y(o)}$ which satisfies the initial problem

$$\begin{cases} \frac{d}{dt}B(t) = FB \\ B(o) = I, \end{cases}$$

where $F(y) = df(y)$ is the derivative of the vector field f. We have

$$\frac{d}{dt}\det B(t) = \det B(t) tr(B^{-1}\frac{d}{dt}B) = \det B(t)\ trF$$

so that phase space volume contracts, conserves or expands when $trF < 0$, $trF = 0$ or $F > 0$ for all y respectively. trF is divergence or trace of the vector field f. Up to now in the field of numerical integration, much work [2]-[7],[9] has been done in maintaining the preservation of phase space volume for source-free dynamical systemes:

$$\frac{dy}{dt} = f(y),\ y \in \Re^n \tag{1.2}$$

which satisfy

$$(div\ f)(y) = \sum_{i=1}^{n} \frac{\partial f_i}{\partial y_i} = 0. \tag{1.3}$$

Definition 1.1. In numerically solving a source-free system (1.2)-(1.3), an one-step scheme is called volume-preserving scheme if, as applied to the source-free systems, the numerical solutions generated by the one-step scheme satisfy the volume-preserving condition

$$\det\left(\frac{\partial y_1}{\partial y_0}\right) = 1. \tag{1.4}$$

* Received.

Already for linear source-free systems of dimension $n \geq 3$, a key Lemma 1 in [2] shows that no standard method can be volume-preserving. This negative result motivates the search for new methods which can maintain the preserving of phase space volume. Up to the present the following approaches are found: First the splitting idea yields an approach, for example, proposed by K.feng & Z.J.Shang [2] which comes from decomposing a source-free voctor field as a finite sum of 2-dimensional Hamcltionian fields for which symplectic Euler formula is used. Second approach comes from using generating function [5]-[7].

For standard method, for example, Runge-Kutta method and so on only some special source-free systems have been discussed [4],[9].

This paper is organized as follows. In Section 2, we aim at perfecting the work of [4]. It is shown that for some special source-free systems symmetric and symplectic Runge-Kutta methods as well as symmetric partitioned RK methods with $\overline{b_i} = b_i, i = 1, \cdots, s$ are volume-preserving. In Section 3, for a general linear dynamical system $\dot{y} = Ly$ first doing exponential transformation, and applying a modified θ-method to the new system generated by the transformation can yield some first-order explicit structure-preserving schemes which satisfy

$\det(\frac{\partial y_1}{\partial y_0}) = e^{htrL}$,and then we compose the first-order schemes into arbitrarily high order explicit symmetric structure-preserving ones. In Section 4, for non-linear dynamical systems $\dot{y} = f(y)$ Feng-Shang first-order volume-preserving scheme can be also constructed starting modified θ - methods and is shown that the scheme is structure-preserving to phase space volume.

2. Volume-preserving scheme for linear system with canonical form

As an example, already discussing in all details [2] linear source-free system in $\Re^3$

$$\begin{cases} \dfrac{dy}{dt} = Ly, & (2.1) \\ trL = 0 & (2.2) \end{cases}$$

solved by trapezied formula will give us valuable enlightenment. First we can get algorithmic approximation G^h to $e_L^h = \exp(hL)$ with

$$G^h = (I - \frac{h}{2}L)^{-1}(I + \frac{h}{2}L),$$

in general, it is scarcely possible that $\det(G^h) = 1$. Now we pay attention to the following fact of the matter:

For matrix $L = (l_{ij})_{i,j=1}^3$ which satisfies $trL = 0$, there exists a reversible matrix P such that the value of $P^{-1}LP$ only takes one of

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & -\lambda_1 & 0 \\ 0 & 0 & \lambda_1 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix},$$

where $\sum_{i=1}^{3} \lambda_i = 0$ and $\prod_{i=1}^{3} \lambda_i = \det(L)$. Obviously, only the first case $(0, -\lambda_1, \lambda_1)$ means that it is possible for the systems (2.1)-(2.2) to be stable, and leads to $\det(G^h) = 1$, i.e. trapezoid formula being volume-preserving. Orther case means that corresponding linear source-free systems (2.1)-(2.2) are not stable (that is, at least, there exists a component of solutions for systems (2.1)-(2.2) being unbounded as $t \to \infty$), and leads to trapezied formula being non-volume-preserving.

Now we extend such discussion to n-dimension linear source-free system.

In many application linear source-free systems (2.1)-(2.2) considered in $\Re^n$ are stable, so there exist reversible matrix P such that

$$P^{-1}LP=\begin{cases}\text{diag }(0,\pm\lambda_1,\cdots,\pm\lambda_{[n/2]})\text{ or diag }(0,\begin{pmatrix}0&-\mu_1\\ \mu_2&0\end{pmatrix},\cdots,\begin{pmatrix}0&-\mu_{n-2}\\ \mu_{n-1}&0\end{pmatrix}),\\ \text{ as } n=\text{add number}\\ \text{diag }(\pm\lambda_1,\cdots,\pm\lambda_{n/2})\text{ or diag }(\begin{pmatrix}0&-\mu_1\\ \mu_2&0\end{pmatrix},\cdots,\begin{pmatrix}0&-\mu_{n-1}\\ \mu_n&0\end{pmatrix})\\ \text{ as } n=\text{even number,}\end{cases} \tag{2.3}$$

if it is not the case, corresponding linear source-free systems (2.1)-(2.2) in $\Re^n$ are not stable and arise rarely in practice, therefore dividing linear source-free systems (2.1)-(2.2) in $\Re^n$ into two categories is reasonable.

Definition 2.1. A linear source-free system (2.1)-(2.2) in $\Re^n$ satisfying the condition (2.3)is called the canonical form of (2.1)-(2.2)(or canonical system), otherwise, non-canonical form (or non-canonical system).

Remark 1. Any stable linear source-free system (2.1)-(2.2) in $\Re^n$ is a canonical system.

Remark 2. If $L$is a real skew-symmetric matrix, then the system (2.1) is a canonical one. This is because under this assumption we can find from matrix theory an orthogonal matrix Q such that

$$Q^TLQ=\begin{cases}\text{diag }(0,\begin{pmatrix}0&\mu_1\\ -\mu_1&0\end{pmatrix},\cdots,\begin{pmatrix}0&\mu_{[n/2]}\\ -\mu_{[n/2]}&0\end{pmatrix}),\ \text{as } n=\text{add number,}\\ \text{diag }(\begin{pmatrix}0&\mu_1\\ -\mu_1&0\end{pmatrix},\cdots,\begin{pmatrix}0&\mu_{n/2}\\ -\mu_{n/2}&0\end{pmatrix}),\ \text{as } n=\text{even number,}\end{cases}$$

where some of the μ_i may be zero.

For initial value problem (2.1) with $y\,|_{t=0}=y_0$ if we perform the transformation $y=Px$ then (2.1) is translated into the initial value problem

$$\begin{cases}\frac{dx}{dt}=P^{-1}LP=\bar{L}x,\ \bar{L}\in\Re^n,\\ x_0=P^{-1}y_0.\end{cases} \tag{2.4}$$

Thus there are

$$\frac{\partial y(t)}{\partial y_0}=P\frac{\partial x(t)}{\partial x_0}P^{-1}$$

and

$$\det\left(\frac{\partial y(t)}{\partial y_0}\right)=\det\left(\frac{\partial \mathrm{x(t)}}{\partial \mathrm{x}_0}\right),$$

where $(\frac{\partial y(t)}{\partial y_0})$ and $(\frac{\partial x(t)}{\partial x_0})$ stand for the Jacobi matrix of solutions of (2.1) and (2.4) respectively.

Remark 3. Applying one-step of a Runge-Kutta method to the initial value problem (2.1) and (2.4) in $\Re^n$ leads to

$$\det\left(\frac{\partial \mathrm{y}_1}{\partial \mathrm{y}_0}\right)=\det\left(\frac{\partial x_1}{\partial x_0}\right). \tag{2.5}$$

A Runge-Kutta method for the solution of (2.1) is given by

$$\begin{cases}X_i=x_0+h\sum\limits_{j=1}^{s}a_{ij}LX_j,\ 1\le i\le s\\ x_1=x_0+h\sum\limits_{i=1}^{s}b_iLX_i.\end{cases} \tag{2.6}$$

Let I_n denotes an $n\times n$ unit matrix, $X=(X_1,\cdots,X_s)^T$, $\bar{A}=A\otimes I_n,\bar{b}=b^T\otimes I_n$ and $e_n=e\otimes I_n$, where the symbol $B\otimes C$ denotes the Kronecker product of the matrices B and C. Thus (2.6) can be written in more compact form

$$\begin{cases}X=e_nx_0+h\bar{A}LX & (2.7a)\\ x_1=x_0+h\bar{b}LX. & (2.7b)\end{cases}$$

This leads straightforwardly to the following expression for the Jacobi matrix of solutions generated by Runge-Kutta method (2.7)

$$\left(\frac{\partial x_1}{\partial x_0}\right) = \left(I_{sn} + h\bar{b}^T L(I_{sn} - h\bar{A}L)^{-1} e_n\right). \tag{2.7}$$

By general knowledge coming from linear algebra (see also [4] or [9]), it is easy to get from (2.7)

$$\det \left(\frac{\partial x_1}{\partial x_0}\right) = \frac{\det \ (I_{sn} + h(eb^T - A) \otimes I_n L)}{\det \ (I_{sn} - h\bar{A}L)}. \tag{2.8}$$

If the Runge-Kutta method is symmetric [8], [11] we can obtain

$$\det \left(\frac{\partial x_1}{\partial x_0}\right) = \frac{\det \ (I_{sn} + h\bar{A}L)}{\det \ (I_{sn} - h\bar{A}L)}. \tag{2.9}$$

By Remark 3 there is

$$\det \left(\frac{\partial x_1}{\partial x_0}\right) = \frac{\det \ (I_{sn} + h\bar{A}L)}{\det \ (I_{sn} - h\bar{A}L)} = \frac{\det \ (I_{sn} + h\bar{A}\bar{L})}{\det \ (I_{sn} - \bar{A}\bar{L})}. \tag{2.9'}$$

where $\bar{L} = P^{-1}LP$.

And since the stability function of symplectic Runge-Kutta methods satisfies [1]

$R(Z)R(-Z) = 1$ for all complex Z,

thus applying symplectic RK to the linear system (2.1) leads also to (2.9). Therefore by Definition 2.1., (2.9) and (2.9)' we can obtain the following result:

Theorem 2.2. For the canonical system (2.1)-(2.2) in $\Re^n$ all symmetric Runge-Kutta methods and symplectic ones are volume-preserving.

The same argument shows that the following result holds also:

Theorem 2.3. For the canonical system (2.1)-(2.2) in $\Re^n$ all symmetric partitioned Runge-Kutta methods with weights $\bar{b}_i = b_i, i = 1, \cdots, s$, are volume-preserving.

Remark 4. For the canonical systems (2.1)-(2.2) in $\Re^n$ non-symmetric symplectic partitioned Runge-Kutta methods are not volume-preserving. For example, it is easy to verify that symplectic Euler formula applied to following canonical system

$$\begin{pmatrix} \frac{dx}{dt} \\ \frac{dy}{dt} \\ \frac{dz}{dt} \end{pmatrix} = \begin{pmatrix} 0 & \frac{mn}{l} & -\frac{mn}{l} \\ -\frac{nl}{m} & 0 & \frac{nl}{m} \\ \frac{ml}{n} & -\frac{ml}{n} & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \tag{2.10}$$

leads to det $\left(\frac{\partial(x_1,y_1,z_1)}{\partial(x_0,y_0,z_0)}\right) \neq 1$.

3. Structure-preserving schemes for linear dynamical systems

If $ODE_S(1.1)$ discussed in Section 1. is linear dynamical systems $\dot{y} = Ly$, $y \in \Re^n$, then Jacabian $B(t) = \frac{\partial y(t)}{\partial y_0} = e^{Lt}$ satisfies obviously the initial value problem

$$\begin{cases} \frac{d}{dt}B(t) = LB(t) \\ B(0) = I \end{cases}$$

and

$$\frac{d}{dt} \ \det \ (B(t)) = \det \ (B(t)) \ \mathrm{tr} \ L.$$

In this section we consider $trL = a, a \in [-b, c]$, where $b,\ c$ are small positive real number. In other words, we consider $-b \le a < 0$ corresponding to weakly contracting phase space volume (non-stiff case), $a = 0$ corresponding to conserving one and $0 < a \leq c$ to corresponding weakly expanding one respectively.

Definition 3.1. In numerical solving a linear dynamical system $\dot{y} = Ly$ an one-step method is called complete structure-preserving scheme if, as applied to the system, the numerical solutions generated, satisfy det $(\frac{\partial y_1}{\partial y_0}) = e^{h\mathrm{tr}\ L}$.

In order to compact length of writing we will straightforward discuss general dynamical system in $\Re^n$

$$\frac{dy}{dt} = f(y), \tag{3.1}$$

Here we consider a class of generalized θ-methods (or modified θ-methods). A modified θ-method for the solution of (3.1) is given by

$$\begin{array}{l} \hat{y}_i = y_i + hf_i(Y_{i1}, \cdots, Y_{in}),\ i = 1, \cdots, n \\ Y_{ij} = \theta_{ij}\hat{y}_j + (1-\theta_{ij})y_j,\ \mathrm{i,j} = 1, \cdots, n \end{array} \tag{3.2}$$

Where y_i and $\hat{y}_i$ are approximations to components $y_i(t_0)$ and $y_i(t_0 + h)$ of exact solutions respectively.

This implies straightforward the following relational expression for the Jacobi matrix of numerical solutions generated by formula (3.2)

$$\begin{array}{l} (\frac{\partial \hat{y}}{\partial y}) = I_n + h \left(\begin{array}{llll} \theta_{11}\frac{\partial f_1}{\partial Y_{11}} & \theta_{12}\frac{\partial f_1}{\partial Y_{12}} & \cdots & \theta_{1n}\frac{\partial f_1}{\partial Y_{1n}} \\ \cdots & & & \\ \theta_{n1}\frac{\partial f_n}{\partial Y_{n1}} & \theta_{n2}\frac{\partial f_n}{\partial Y_{n2}} & \cdots & \theta_{nn}\frac{\partial f_n}{\partial Y_{nn}} \end{array} \right) (\frac{\partial \hat{y}}{\partial y}) \\ +h \left(\begin{array}{llll} (1-\theta_{11})\frac{\partial f_1}{\partial Y_{11}} & (1-\theta_{12})\frac{\partial f_1}{\partial Y_{12}} & \cdots & (1-\theta_{1n})\frac{\partial f_1}{\partial Y_{1n}} \\ \cdots & & & \\ (1-\theta_{n1})\frac{\partial f_n}{\partial Y_{n1}} & (1-\theta_{n2})\frac{\partial f_n}{\partial Y_{n2}} & \cdots & (1-\theta_{nn})\frac{\partial f_n}{\partial Y_{nn}} \end{array} \right), \end{array} \tag{3.3}$$

And leads to

$$\det\ (\frac{\partial \hat{y}}{\partial y}) = \frac{D_n(n)}{D_d(n)}, \tag{3.4}$$

where

$$D_n(n) = \det \left(\begin{array}{llll} 1 + h(1-\theta_{11})\frac{\partial f_1}{\partial Y_{11}} & h(1-\theta_{12})\frac{\partial f_1}{\partial Y_{12}} & \cdots & h(1-\theta_{1n})\frac{\partial f_1}{\partial Y_{1n}} \\ h(1-\theta_{21})\frac{\partial f_2}{\partial Y_{21}} & 1 + h(1-\theta_{22})\frac{\partial f_2}{\partial Y_{22}} & \cdots & h(1-\theta_{2n})\frac{\partial f_2}{\partial Y_{2n}} \\ \cdots & & & \\ h(1-\theta_{n1})\frac{\partial f_n}{\partial Y_{n1}} & h(1-\theta_{n2})\frac{\partial f_n}{\partial Y_{n2}} & \cdots & 1 + h(1-\theta_{nn})\frac{\partial f_n}{\partial Y_{nn}} \end{array} \right). \tag{3.5}$$

and

$$D_d(n) = \det \left(\begin{array}{llll} 1 - h\theta_{11}\frac{\partial f_1}{\partial Y_{11}} & -h\theta_{12}\frac{\partial f_1}{\partial Y_{12}} & \cdots & -h\theta_{1n}\frac{\partial f_1}{\partial Y_{1n}} \\ -h\theta_{21}\frac{\partial f_2}{\partial Y_{21}} & 1 - h\theta_{22}\frac{\partial f_2}{\partial Y_{22}} & \cdots & -h\theta_{2n}\frac{\partial f_2}{\partial Y_{2n}} \\ \cdots & & & \\ -h\theta_{n1}\frac{\partial f_n}{\partial Y_{n1}} & -h\theta_{n2}\frac{\partial f_n}{\partial Y_{n2}} & \cdots & 1 - h\theta_{nn}\frac{\partial f_n}{\partial Y_{nn}} \end{array} \right). \tag{3.6}$$

In formulas (3.4) taking

$$\left\{ \begin{array}{ll} \theta_{ij} = 0 & \text{as}\ \ j > i \\ \theta_{ij} = 1 & \text{as}\ \ j < i \end{array} \right. \tag{3.7}$$

leads to

$$\det\ (\frac{\partial \hat{y}}{\partial y}) = \frac{\prod_{i=1}^{n} (1 + h(1-\theta_{ii})\frac{\partial f_i}{\partial Y_{ii}})}{\prod_{i=1}^{n} (1 - h\theta_{ii}\frac{\partial f_i}{\partial Y_{ii}})}. \tag{3.8}$$

Thus we can obtain from (3.8) the following results:

Case 1. For system (3.1) if condition (3.7) and $\frac{\partial f_i}{\partial y_i}=0,(i=1,\cdots,n)$ hold, then (3.8) becomes det $(\frac{\partial \hat{y}}{\partial y})=1$,this yields (also see [2],[3]) the following first-order explicit volume-preserving scheme

$$\begin{cases} \hat{y}_1 = y_1 + hf_1(y_2,\cdots,y_n) \\ \hat{y}_j = y_j + hf_j(\hat{y}_1,\cdots,\hat{y}_{j-1},y_{j+1},\cdots,y_n), j=2,\cdots,n-1 \\ \hat{y}_n = y_n + hf_n(\hat{y}_1,\cdots,\hat{y}_{n-1}). \end{cases} \tag{3.9}$$

Case 2. For system (3.1) if condition (3.7) and $\frac{\partial f_i}{\partial y_i}=0, i=1,\cdots,(n-2),(\frac{\partial f_{n-1}}{\partial y_{n-1}}+\frac{\partial f_n}{\partial y_n}=0)$ hold, taking $\theta_{n-1,n-1}=1$ and $\theta_{nn}=0$ leads to the following Volume-preserving scheme

$$\begin{cases} \hat{y}_1 = y_1 + hf_1(y_2,\cdots,y_n) \\ \hat{y}_j = y_j + hf_j(\hat{y}_1,\cdots,\hat{y}_{j-1},y_{j+1},\cdots,y_n),\ j=2,\cdots,(n-2) \\ \hat{y}_{n-1} = y_{n-1} + hf_{n-1}(\hat{y}_1,\cdots,\hat{y}_{n-1},y_n) \\ \hat{y}_n = y_n + hf_n(\hat{y}_1,\cdots,\hat{y}_{n-1},y_n) \end{cases} . \tag{3.10}$$

Case 3. Consider the following perturbed problem

$$\begin{cases} \frac{dy_1}{dt} = a_1 y_1 + f_1(y_2,\cdots,y_n) \\ \frac{dy_i}{dt} = a_i y_i + f_i(y_1,\cdots,y_{i-1},y_{i+1},\cdots,y_n),\ i=2,\cdots,n-1 \\ \frac{dy_n}{dt} = a_n y_n + f_n(y_1,\cdots,y_{n-1}) \end{cases} \tag{3.11}$$

where $\sum_{i=1}^{n} a_i = a,\ -b \le a \le c$, under transformation $y_i = e^{a_i t}u_i,\ i=1,\cdots,n$, a new source-free system $\frac{du}{dt}=\bar{f}(u,t)$ with $\frac{\partial \bar{f}_i}{\partial u_i}=0,\ i=1,\cdots,n$ is derived. Thus the scheme (3.9) applied to the new system leads to the following first-order explicit structure-preserving schemes

$$\begin{cases} \hat{y}_1 = e^{a_1 h}\{y_1 + hf_1(y_2,\cdots,y_n)\} \\ \hat{y}_j = e^{a_j h}\{y_j + hf_j(\hat{y}_1,\cdots,\hat{y}_{j-1},y_{j+1},\cdots,y_n)\},\ j=2,\cdots,n-1 \\ \hat{y}_n = e^{a_n h}\{y_n + hf_n(\hat{y}_1,\cdots,\hat{y}_{n-1})\} \end{cases} \tag{3.12}$$

and

$$\begin{cases} \hat{y}_1 = e^{a_1 h}y_1 + hf_1(y_2,\cdots,y_n) \\ \hat{y}_j = e^{a_j h}y_j + hf_j(\hat{y}_1,\cdots,\hat{y}_{j-1},y_{j+1},\cdots,y_n),\ j=2,\cdots,n-1 \\ \hat{y}_n = e^{a_n h}y_n + hf_n(\hat{y}_1,\cdots,\hat{y}_{n-1})\ . \end{cases} \tag{3.13}$$

In particular for linear dynamical system

$$\frac{dy}{dt} = Ly,\ trL = a,\ y \in \Re^n \tag{3.14}$$

it follows from case 3 that

Theorem 3.2. For linear dynanical system (3.14) Both schemes (3.12) and (3.13) are complete structure-preserving.

Remark 5. By approach of [2] (also see [3],[10]), for linear system (3.14) schemes (3.12) and (3.13), for example, scheme (3.12) can be composed into explicit symmetric complete structure-preserving one of order 2, as follows

$$\begin{cases} \hat{y}_n^{1/2} = e^{\frac{1}{2}ha_n}\left\{y_n + \frac{h}{2}f_n(y_1,\cdots,y_{n-1})\right\} \\ \hat{y}_j^{1/2} = e^{\frac{1}{2}ha_j}\left\{y_j + \frac{h}{2}f_j(y_1,\cdots,y_{j-1},\hat{y}_{j+1}^{1/2},\cdots,\hat{y}_n^{1/2})\right\},\ j=n-1,\cdots,2 \\ \hat{y}_1^{1/2} = e^{\frac{1}{2}ha_1}\left\{y_1 + \frac{h}{2}f_1(\hat{y}_2^{1/2},\cdots,\hat{y}_n^{1/2})\right\} \\ \hat{y}_1 = e^{\frac{h}{2}a_1}\left\{\hat{y}_1^{1/2} + \frac{h}{2}f_1(\hat{y}_2^{1/2},\cdots,\hat{y}_n^{1/2})\right\} \\ \hat{y}_j = e^{\frac{1}{2}ha_j}\left\{\hat{y}_j^{1/2} + \frac{h}{2}f_j(\hat{y}_1,\cdots,\hat{y}_{j-1},\hat{y}_{j+1}^{1/2},\cdots,\hat{y}_n^{1/2})\right\},\ j=2,\cdots,n-1 \\ \hat{y}_n = e^{\frac{1}{2}ha_n}\left\{\hat{y}_n^{1/2} + \frac{h}{2}f_n(\hat{y}_1,\cdots,\hat{y}_{n-1})\right\}. \end{cases} \tag{3.15}$$

Remark 6. We start from the basic scheme (3.15), by Yashida's approach [12] (also see [2]) arbitrarily high order explicit symmetric complete structure-preserving schemes can be constructed.

4. Structure-preserving schemes for non-linear dynamical systems

For non-linear dynamical systems (3.1)

$$\frac{dy}{dt} = f(y)$$

we discuss again the modified θ - methods for the solution of (3.1) and repeat the argument in Section 3 (from general expression (3.2) to the condition (3.7)). Finally we obtain

$$\det\left(\frac{\partial \hat{y}}{\partial y}\right) = \frac{\prod_{i=1}^{n}\left(1 + h(1-\theta_{ii})\frac{\partial f_i}{\partial Y_{ii}}\right)}{\prod_{i=1}^{n}\left(1 - h\theta_{ii}\frac{\partial f_i}{\partial Y_{ii}}\right)}. \tag{4.1}$$

Obviously if $\frac{\partial f_i}{\partial y_i} \neq 0, i = 1, 2, ..., n, n \geq 3$ then for any $\theta_{ii}, i = 1, 2, ..., n$

$$\det\left(\frac{\partial \hat{y}}{\partial y}\right) \neq 1.$$

Taking $n = 3,\ \theta_{11} = \theta_{22} = 1$ and $\theta_{33} = 0$ lead to

$$\begin{cases} \hat{y}_1 = y_1 + hf_1(\hat{y}_1, y_2, y_3) & (4.3a) \\ \hat{y}_2 = y_2 + hf_2(\hat{y}_1, \hat{y}_2, y_3) & (4.3b) \\ \hat{y}_3 = y_3 + hf_3(\hat{y}_1, \hat{y}_2, y_3) & (4.3c) \end{cases}$$

and

$$\det\left(\frac{\partial \hat{y}}{\partial y}\right) = \frac{(1 + h\frac{\partial}{\partial y_3} f_3(\hat{y}_1, \hat{y}_2, y_3))}{(1 - h\frac{\partial f_1}{\partial y_1}(\hat{y}_1, y_2, y_3))(1 - h\frac{\partial}{\partial y_2} f_2(\hat{y}_1, \hat{y}_2, y_3))}. \tag{4.4}$$

Now we modify (4.3b) in (4.3) such that

$$\hat{y}_2 = y_2 + hf_2(\hat{y}_1, \hat{y}_2, y_3) + h\int_{y_2}^{\hat{y}_2} \frac{\partial}{\partial y_1} f_1(\hat{y}_1, y, y_3)dy \tag{4.3b'}$$

and then can get

$$\begin{aligned} \det\left(\frac{\partial \hat{y}}{\partial y}\right) &= \frac{(1-h\frac{\partial f_1}{\partial y_1}(\hat{y}_1, y_2, y_3))(1+h\frac{\partial f_3}{\partial y_3}(\hat{y}_1, \hat{y}_2, y_3))}{(1-h\frac{\partial f_1}{\partial y_1}(\hat{y}_1, y_2, y_3))[1-h(\frac{\partial f_1}{\partial y_1}(\hat{y}_1, \hat{y}_2, y_3)+\frac{\partial f_2}{\partial y_2}(\hat{y}_1, \hat{y}_2, y_3))]} \\ &= \frac{(1+h\frac{\partial f_3}{\partial y_3}(\hat{y}_1, \hat{y}_2, y_3))}{[1-h(\frac{\partial f_1}{\partial y_1}(\hat{y}_1, \hat{y}_2, y_3)+\frac{\partial f_2}{\partial y_2}(\hat{y}_1, \hat{y}_2, y_3))]}. \end{aligned} \tag{4.5}$$

Let $\sum_{i=1}^{n} \frac{\partial f_1}{\partial y_i} = a, n \geq 3$ we can get first-order Feng-Shang scheme [2]

$$\begin{cases} \hat{y}_1 = y_1 + hf_1(\hat{y}_1, y_2, \cdots, y_n) \\ \hat{y}_j = y_j + hf_j(\hat{y}_1, \cdots, \hat{y}_j, y_{j+1}, \cdots, y_n) + h\int_{y_j}^{\hat{y}_j} \sum_{l=1}^{j-1} \frac{\partial f_l}{\partial y_l}(\hat{y}_1, \cdots, \hat{y}_{j-1}, y, y_{j+1}, \cdots, y_n)dy \\ \ j = 2, \cdots, n-1 \\ \hat{y}_n = y_n + hf_n(\hat{y}_1, \hat{y}_2, \cdots, \hat{y}_{n-1}, y_n) \end{cases} \tag{4.6}$$

and

$$\det(\frac{\partial \hat{y}}{\partial y}) = \frac{(1 + h\frac{\partial f_n}{\partial y_n}(\hat{y}_1, \cdots, \hat{y}_{n-1}, y_n))}{(1 - h\sum_{i=1}^{n-1} \frac{\partial f_i}{\partial y_i}(\hat{y}_1, \hat{y}_2, \cdots, \hat{y}_{n-1}, y_n))}$$

$$= \frac{(1 + h\frac{\partial f_n}{\partial y_n}(\hat{y}_1, \cdots, \hat{y}_{n-1}, y_n))}{[1 + h(\frac{\partial f_n}{\partial y_n}(\hat{y}_1, \cdots, \hat{y}_{n-1}, y_n) - a)]}. \tag{4.7}$$

It follows from (4.7) that

Theorem 4.1. For non-linear dynamical systems (3.1),

i) first-order Feng-Shang scheme (4.6) is Volume-preserving when $a = 0$;

ii) the scheme is contracting to phase space volume when $a < 0$;

iii) the scheme is expanding to phase space volume when $a > 0$.

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