Numer. Math. 71: 451–463 (1995)

Numerische
Mathematik

Volume-preserving algorithms for source-free dynamical systems*

Feng Kang[1], **Shang Zai-jiu**[2]

[1] Computing Center, Academia Sinica, Beijing 100080, China
[2] Institute of Mathematics, Academia Sinica, Beijing 100080, China, Fax: 86-1-2568356

Received March 22, 1994 / Revised version received January 25, 1995

Summary. In this paper, we first expound why the volume-preserving algorithms are proper for numerically solving source-free systems and then prove all the conventional methods are not volume-preserving. Secondly, we give a general method of constructing volume-preserving difference schemes for source-free systems on the basis of decomposing a source-free vector field as a finite sum of essentially 2-dimensional Hamiltonian fields and of composing the corresponding essentially symplectic schemes into a volume-preserving one. Lastly, we make some special discussions for so-called separable source-free systems for which arbitrarily high order explicit revertible volume-preserving schemes can be constructed.

Mathematics Subject Classification (1991): 65L05, 34A50

1 Introduction

Source-free dynamical systems on the Euclidean space $\mathbb{R}^n$ are defined by source-free (or divergence-free) vector fields $a : \mathbb{R}^n \to \mathbb{R}^n$,

$$(1.1)\qquad (\operatorname{div} a)(x) = \sum_{i=1}^{n} \frac{\partial a_i}{\partial x_i}(x) = 0 \quad \text{identically for } x \in \mathbb{R}^n$$

through equations

$$(1.2)\qquad \frac{dx}{dt} = \dot{x} = a(x).$$

Here and hereafter we use the coordinate description and matrix notation:

* Project supported by State Commission of Science and Technology of China
Correspondence to: Z.-J. Shang

$$x = (x_1, \cdots, x_n)^{\mathrm{T}}, \quad a(x) = (a_1(x), \cdots, a_n(x))^{\mathrm{T}}, \tag{1.3}$$

where T denotes the transpose of matrix.

In this paper we mainly analyse and construct numerical algorithms proper for source-free systems. Such systems constitute one of the most important classical cases of dynamical systems preserving certain geometric structure and arise in many physical problems such as particle tracking in incompressible fluids and toroidal magnetic surface-generating in stellarators. Since the difficulty and even impossibility of solving equations by quadrature, the numerical methods certainly play an important role in understanding the dynamic behavior of a system and in solving physical and engineering problems. On the other hand, the problem of whether a numerical algorithm is proper for a system is closely related to the problem of whether the algorithmic approximation to the corresponding phase flow approximates perfectly in some sense and even strictly preserve the structure of the system itself if the system has such structure. It has been evidenced with some typical examples in the Hamiltonian case that "nonproper" algorithms will result in essentially wrong approximations to the solutions of systems and "proper" algorithms may generate remarkably right ones [2].

But how does one evaluate a numerical algorithm to be proper for source-free systems? It is well known that intrinsic to all source-free systems, there is a volume form of the phase space $\mathbb{R}^n$, say

$$\alpha = dx_1 \wedge dx_2 \wedge \cdots \wedge dx_n, \tag{1.4}$$

such that the evolution of dynamics preserve this form. In other words, the phase flow e_a^t, of source-free system (1.2), satisfies the volume-preserving condition

$$(e_a^t)^* \alpha = \alpha, \tag{1.5}$$

or equivalently,

$$\det \frac{\partial e_a^t}{\partial x}(x) = 1 \quad \text{identically for } x \in \mathbb{R}^n \text{ and } t \in \mathbb{R}. \tag{1.5$'$}$$

In addition to this, e_a^t satisfies the group property in t

$$e_a^0 = \text{identity}, \quad e_a^{t+s} = e_a^t \circ e_a^s. \tag{1.6}$$

In fact, (1.5) and (1.6) completely describe the properties of the most general source-free dynamical systems. This fact suggests that a proper algorithmic approximation g_a^s to phase flow e_a^s for source-free vector field $a : \mathbb{R}^n \to \mathbb{R}^n$ should satisfy these two requirements. However, the group property (1.6) is too stringent in general for algorithmic approximations because only the phase flows satisfy it. Instead of it, a weaker requirement

$$g_a^0 = \text{identity}, \quad g_a^s \circ g_a^{-s} = \text{identity} \tag{1.7}$$

is reasonable and practicable for all vector fields $a : \mathbb{R}^n \to \mathbb{R}^n$ (see for example [4]). We call such algorithmic approximations revertible, that means g_a^s always generate coincident forward and backward orbits. As for the volume-preserving property (1.5), it characterizes the geometric structure – volume-preserving structure – of source-free systems. Our aim in this paper is just to construct difference schemes preserving this structure, which we call volume-preserving schemes, in the sense that the algorithmic approximations to the phase flows satisfy (1.5) for the most general source-free systems.

2 Obstruction to analytic methods

We note that for $n = 2$, source-free vector fields = Hamiltonian fields, and area-preserving maps = symplectic maps, so the problem for area-preserving algorithms has been solved in principle [5].

But for $n \geq 3$, the problem is new, since all the conventional methods plus even the symplectic methods are generally not volume-preserving, even for linear source-free systems. As an illustration, solve on $\mathbb{R}^3$

$$\frac{dx}{dt} = a(x) = Ax, \quad \mathrm{tr}A = 0 \tag{2.1}$$

by the Euler centered method, we get algorithmic approximation G^s to $e_a^s = \exp(sA)$ with

$$G^s = (I - \frac{s}{2}A)^{-1}(I + \frac{s}{2}A). \tag{2.2}$$

Simple calculations show that in 3-dimensions, if $\mathrm{tr}A = 0$, then $\det G^s = 1 \Leftrightarrow \det A = 0$, which is exceptional. A more general conclusion in linear case is

Lemma 1 *Let $sl(n)$ denote the set of all $n \times n$ real matrices with trace equal to zero and $SL(n)$ the set of all $n \times n$ real matrices with determinant equal to one. Then for any real analytic function $\phi(z)$ defined in a neighbourhood of $z = 0$ in $\mathbb{C}$ satisfying the conditions:* 1) $\phi(0) = 1$ *and* 2) $\phi'(0) = 1$, *we have that $\phi(sl(n)) \subset SL(n)$ for some $n \geq 3$ if and only if $\phi(z) = \exp(z)$.*

Proof. "If part" is a known conclusion. For the "only if part" it suffices to show it for $n = 3$. For this, we consider matrices of the diagonal form

$$D(s,t) = \begin{pmatrix} s & 0 & 0 \\ 0 & t & 0 \\ 0 & 0 & -(s+t) \end{pmatrix} \in sl(3), \quad s,t \in \mathbb{R}. \tag{2.3}$$

Since ϕ is analytic in a neighbourhood of the origin in $\mathbb{C}$, we have

$$\phi(D(s,t)) = \begin{pmatrix} \phi(s) & 0 & 0 \\ 0 & \phi(t) & 0 \\ 0 & 0 & \phi(-(s+t)) \end{pmatrix}, \quad s,t \sim 0. \tag{2.4}$$

By assumption, $\det\phi(D(s,t)) = 1$ for $s,t \sim 0$. So,

$$\phi(s)\phi(t)\phi(-(s+t)) = 1, \quad s,t \sim 0. \tag{2.5}$$

This together with the condition $\phi(0) = 1$ yields

$$\phi(s)\phi(-s) = 1, \quad s \sim 0. \tag{2.6}$$

Multiplying the both sides of Eq. (2.5) by $\phi(s+t)$ and using (2.6), we get

$$\phi(s)\phi(t) = \phi(s+t), \quad s, t \sim 0. \tag{2.7}$$

This, together with the conditions 1) and 2) of the lemma, implies

$$\phi(z) = \exp(z)$$

which completes the proof. □

Lemma 1 says that there are no consistent analytic approximations to the exponential function sending at the same time $sl(n)$ into $SL(n)$ other than the exponential itself. This shows that it is impossible to construct volume-preserving algorithms analytically depending on source-free vector fields. Thus we have

Theorem 1 *All the conventional methods including the well-known Runge-Kutta methods, linear multistep methods and Euler methods (explicit, implicit and centered) are non-volume-preserving.*

Consequently, to construct volume-preserving algorithms for source-free systems, we must break through the conventional model and explore new ways.

3 "Essentially Hamiltonian decompositions" of source-free vector fields

In $\mathbb{R}^2$, every source-free field $a = (a_1, a_2)^{\mathrm{T}}$ corresponds to a stream function or 2-dimensional Hamiltonian ψ, unique up to a constant:

$$a_1 = -\frac{\partial\psi}{\partial x_2}, \quad a_2 = \frac{\partial\psi}{\partial x_1}; \tag{3.1}$$

and in $\mathbb{R}^3$, every source-free field $a = (a_1, a_2, a_3)^{\mathrm{T}}$ corresponds to a vector potential $b = (b_1, b_2, b_3)^{\mathrm{T}}$, unique up to a gradient:

$$a = \mathrm{curl} b, \quad a_1 = \frac{\partial b_3}{\partial x_2} - \frac{\partial b_2}{\partial x_3}, a_2 = \frac{\partial b_1}{\partial x_3} - \frac{\partial b_3}{\partial x_1}, a_3 = \frac{\partial b_2}{\partial x_1} - \frac{\partial b_1}{\partial x_2}, \tag{3.2}$$

then we get source-free decomposition

$$a = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} 0 \\ \frac{\partial b_1}{\partial x_3} \\ -\frac{\partial b_1}{\partial x_2} \end{pmatrix} + \begin{pmatrix} -\frac{\partial b_2}{\partial x_3} \\ 0 \\ \frac{\partial b_2}{\partial x_1} \end{pmatrix} + \begin{pmatrix} \frac{\partial b_3}{\partial x_2} \\ -\frac{\partial b_3}{\partial x_1} \\ 0 \end{pmatrix} = a^{(1)} + a^{(2)} + a^{(3)}. \tag{3.3}$$

As a generalization of cases $n = 2, 3$, on $\mathbb{R}^n$, we have

Lemma 2 *To every source-free field $a = (a_1, a_2, \cdots, a_n)^{\mathrm{T}}$, there corresponds a skew symmetric tensor field of order 2, $b = (b_{ik})_{1 \le i,k \le n}$, $b_{ik} = -b_{ki}$, so that*

$$a_i = \sum_{k=1}^{n} \frac{\partial b_{ik}}{\partial x_k}, \quad i = 1, 2, \cdots, n. \tag{3.4}$$

Proof. [1] With the given $a = (a_1, \cdots, a_n)^{\mathrm{T}}$, we define the 1-form on $\mathbb{R}^n$

$$\alpha = \sum_{i=1}^{n} a_i(x) dx_i . \tag{3.5}$$

Since a is source-free, we have $\delta\alpha = -\sum_{i=1}^{n} \frac{\partial a_i}{\partial x_i} = -\mathrm{div} a = 0$, which means that α is δ-closed. By Poincaré's lemma, there exists a 2-form, say β, so that

$$\alpha = \delta\beta. \tag{3.6}$$

But for the 2-form β, there exists a skew symmetric tensor of order 2, $b = (b_{ik})_{1\le i.k\le n}$, $b_{ik} = -b_{ki}$, so that

$$\beta = \sum_{i,k=1}^{n} b_{ik} dx_i \wedge dx_k . \tag{3.7}$$

Seeing that

$$\delta\beta = \sum_{i=1}^{n} \Big(\sum_{k=1}^{n} \frac{\partial b_{ik}}{\partial x_k} \Big) dx_i \tag{3.8}$$

and noticing Eqs. (3.5) and (3.6), we get (3.4). The proof is completed.

By (3.4), we can decompose

$$a = \sum_{1\le i<k\le n} a^{(ik)}, \quad a^{(ik)} = \Big(0, \cdots, 0, \frac{\partial b_{ik}}{\partial x_k}, 0, \cdots, -\frac{\partial b_{ik}}{\partial x_i}, 0, \cdots, 0\Big)^{\mathrm{T}}, i < k. \tag{3.9}$$

Every vector field $a^{(ik)}$ in (3.9) is 2-dimensional Hamiltonian on the x_i-x_k plane and zero in other dimensions. We call such decompositions essentially Hamiltonian decompositions.

We note that the tensor potential $b = (b_{ik})_{1\le i,k\le n}$ is far from uniquely determined for a given source-free field $a = (a_1, \cdots, a_n)^{\mathrm{T}}$ from Eq. (3.4). For uniqueness one may impose normalizing conditions in many different ways. One way is to impose, as was done by H. Weyl in [17] in 3-dimensional case,

$$N_0 : b_{ik} = 0, \quad |i - k| \ge 2, \tag{3.10}$$

(this condition is ineffective for $n = 2$). The non-zero components are

$$b_{12} = -b_{21}, b_{23} = -b_{32}, \cdots, b_{n-1,n} = -b_{n,n-1}. \tag{3.11}$$

$$N_k : b_{k,k+1}|_{x_{k+1}=0} = 0, 1 \le k \le n-2, \tag{3.12}$$

(this condition is ineffective for $n = 2$).

$$N_{n-1} : b_{n-1,n}|_{x_{n-1}=x_n=0} = 0. \tag{3.13}$$

[1] For the definition of the operator δ, see [16], p.220; for the Poincaré's lemma for the exterior differential operator d, see [10], from which the Poincaré's lemma for the operator δ is easily derived

Then simple calculations show that all $b_{k,k+1}$ are uniquely determined by quadrature

$$(3.14)_1 \qquad b_{12} = \int_0^{x_2} a_1 dx_2,$$

$$(3.14)_k \qquad b_{k,k+1} = \int_0^{x_{k+1}} \left(a_k + \frac{\partial b_{k-1,k}}{\partial x_{k-1}}\right) dx_{k+1}, 2 \leq k \leq n-2,$$

$$(3.14)_{n-1} \qquad b_{n-1,n} = \int_0^{x_n} (a_{n-1} + \frac{\partial b_{n-2,n-1}}{\partial x_{n-2}}) dx_n - \int_o^{x_{n-1}} a_n|_{x_n=0} dx_{n-1}.$$

So one gets an essentially Hamiltonian decomposition for a

$$(3.15) \qquad a = \sum_{k=1}^{n-1} a^{(k)}, \quad a^{(k)} = (0, \cdots, 0, \frac{\partial b_{k,k+1}}{\partial x_{k+1}}, -\frac{\partial b_{k,k+1}}{\partial x_k}, 0, \cdots, 0)^{\mathrm{T}},$$

or in components,

$$(3.15)' \qquad \begin{aligned} a_1 &= \frac{\partial b_{12}}{\partial x_2}, a_2 = -\frac{\partial b_{12}}{\partial x_1} + \frac{\partial b_{23}}{\partial x_3}, \cdots, a_{n-1} \\ &= -\frac{\partial b_{n-2,n-1}}{\partial x_{n-2}} + \frac{\partial b_{n-1,n}}{\partial x_n}, a_n = -\frac{\partial b_{n-1,n}}{\partial x_{n-1}}. \end{aligned}$$

4 Construction of volume-preserving difference schemes

In this section, we give a general way to construct volume-preserving difference schemes for source-free systems by means of the essentially Hamiltonian decompositions of source-free vector fields and the symplectic difference schemes for 2-dimensional Hamiltonian systems. For this aim, we first prove

Lemma 3 *Let a be a smooth vector field on $\mathbb{R}^n$ and have decomposition*

$$(4.1) \qquad a = \sum_{i=1}^{m} a^{(i)}$$

with smooth fields $a^{(i)} : \mathbb{R}^n \to \mathbb{R}^n$, $i = 1, \cdots, m$. Suppose that, for each $i = 1, \cdots, m$, G_i^τ is an approximation of order p to $e^\tau_{a^{(i)}}$, the phase flow of the system associated to the field $a^{(i)}$, in the sense that $\lim_{\tau\to 0} \frac{1}{\tau^p}(G_i^\tau(x) - e^\tau_{a^{(i)}}(x)) = 0$ for all $x \in \mathbb{R}^n$ with some $p \geq 1$. Then we have

(1) for any permutation $(i_1 i_2 \cdots i_m)$ of $(12 \cdots m)$, the compositions

$$(4.2) \qquad {}_1G^\tau_{i_1 i_2 \cdots i_m} := G^\tau_{i_m} \circ \cdots \circ G^\tau_{i_2} \circ G^\tau_{i_1}, \quad {}_1\hat{G}^\tau_{i_1 i_2 \cdots i_m} := \left({}_1G^{-\tau}_{i_1 i_2 \cdots i_m}\right)^{-1}$$

are approximations, of order one, to e^τ_a; and the compositions

$$(4.2)' \qquad {}_2g^\tau_{i_1 i_2 \cdots i_m} := {}_1\hat{G}^{\tau/2}_{i_1 i_2 \cdots i_m} \circ {}_1G^{\tau/2}_{i_1 i_2 \cdots i_m}, \quad {}_2\hat{g}^\tau_{i_1 i_2 \cdots i_m} = {}_1G^{\tau/2}_{i_1 i_2 \cdots i_m} \circ {}_1\hat{G}^{\tau/2}_{i_1 i_2 \cdots i_m}$$

are revertible approximations, of order 2, to e_a^τ*;*

(2) if, for each $i = 1, 2, \cdots, m$, G_i^τ *is an approximation, of order 2, to* e_a^τ*, then*

$$(4.3)\qquad {}_2G^\tau_{i_1 i_2\cdots i_m} := G_{i_m}^{\tau/2}\circ\cdots\circ G_{i_2}^{\tau/2}\circ G_{i_1}^{\tau/2}\circ G_{i_1}^{\tau/2}\circ G_{i_2}^{\tau/2}\circ\cdots\circ G_{i_m}^{\tau/2}$$

is an approximation, of order 2, to e_a^τ*; and it is revertible if each* G_i^τ *is revertible;*

(3) if ${}_2G^\tau$ *is a revertible approximation, of order 2, to* e_a^τ*, then the symmetric composition*

$$(4.4)_1\qquad {}_4G^\tau = {}_2G^{\alpha_1\tau}\circ {}_2G^{\beta_1\tau}\circ {}_2G^{\alpha_1\tau}$$

with

$$(4.4)'_1\qquad \alpha_1 = (2-2^{1/3})^{-1}, \beta_1 = 1-2\alpha_1 < 0$$

is a revertible approximation, of order 4, to e_a^τ*; and generally, the symmetric composition, recursively defined as follows,*

$$(4.4)_l\qquad {}_{2(l+1)}G^\tau = {}_{2l}G^{\alpha_l\tau}\circ {}_{2l}G^{\beta_l\tau}\circ {}_{2l}G^{\alpha_l\tau}$$

with

$$(4.4)'_l\qquad \alpha_l = (2-2^{1/(2l+1)})^{-1}, \beta_l = 1-2\alpha_l < 0$$

is a revertible approximation, of order $2(l+1)$*, to* e_a^τ*.*

Proof. It is only needed to prove the lemma for $(i_1 i_2\cdots i_m) = (12\cdots m)$.

(1) It is easy to prove that the phase flow e_a^t has the series expansion

$$(4.5)\qquad e_a^t(x) = x + \sum_{k=1}^{\infty}\frac{t^k}{k!}a^k(x),\quad x\in\mathbb{R}^n, t\sim 0,$$

where

(4.6)

$$a^1(x) = a(x),\quad a^2(x) = \frac{\partial a^1}{\partial x}(x)a(x),\quad a^k(x) = \frac{\partial a^{k-1}}{\partial x}(x)a(x),\quad k = 1, 2, \cdots.$$

The assumption that for $i = 1, 2, \cdots, m$, G_i^τ are approximations of order $p\ge 1$, to $e^\tau_{a^{(i)}}$ implies that for all $x\in\mathbb{R}^n$,

$$(4.7)\qquad G_i^\tau(x) = x + \tau a^{(i)}(x) + 0(\tau^2),\quad \tau\sim 0;\quad i = 1, 2, \cdots, m.$$

So, from Taylor expansion, we have that for $x\in\mathbb{R}^n$,

$$(4.8)\quad (G_2^\tau\circ G_1^\tau)(x) = G_2^\tau\left(G_1^\tau(x)\right) = x + \tau(a^{(1)}(x) + a^{(2)}(x)) + 0(\tau^2),\quad \tau\sim 0.$$

By induction for m, we get

$$(4.9)\qquad \begin{aligned} {}_1G^\tau_{(12\cdots m)}(x) &= (G_m^\tau\circ\cdots\circ G_2^\tau\circ G_1^\tau)(x)\\ &= x + \tau(a^{(1)}(x) + a^{(2)}(x) + \cdots a^{(m)}(x)) + 0(\tau^2)\\ &= x + \tau a(x) + 0(\tau^2),\quad \tau\sim 0.\end{aligned}$$

This implies that ${}_1G^{\tau}_{(12\cdots m)}$ is an approximation, of order one, to e^{τ}_a. It was proved in [6] that ${}_2g^{\tau}_{i_1i_2\cdots i_m}$ and ${}_2\hat{g}^{\tau}_{i_1i_2\cdots i_m}$, defined by Eq. (4.2)′, are revertible approximations, of order 2, to e^{τ}_a. The conclusion (1) of the lemma is proved.

(2) By assumption, we have that for $x \in \mathbb{R}^n$ and $\tau \sim 0$,

$$G^{\tau}_i(x) = x + \tau a^{(i)}(x) + \frac{1}{2}\tau^2\left(a^{(i)}\right)^2(x) + 0(\tau^3), \quad i = 1, 2, \cdots, m. \tag{4.10}$$

Taylor expansion of the right hand side of Eq. (4.3) with $(i_1 i_2 \cdots i_m) = (12 \cdots m)$ yields

$${}_2G^{\tau}_{(12\cdots m)}(x) = x + \tau\sum_{i=1}^{m} a^{(i)}(x) + \frac{1}{2}\tau^2\Big(\sum_{i,j=1}^{m} a^{(i)}a^{(j)}\Big)(x) + 0(\tau^3), \quad \tau \sim 0. \tag{4.11}$$

Here we have used the convention

$$(ab)(x) = (a_*b)(x) = a_*(x)b(x), \quad a_*(x) = \frac{\partial a}{\partial x}(x) \tag{4.12}$$

for $a, b : \mathbb{R}^n \to \mathbb{R}^n$. On the other hand, we have

$$a^2 = a_*a = \Big(\sum_{i=1}^{m} a^{(i)}\Big)_*\Big(\sum_{k=1}^{m} a^{(j)}\Big) = \sum_{i,j=1}^{m}(a^{(i)})_*a^{(j)} = \sum_{i,j=1}^{m} a^{(i)}a^{(j)}. \tag{4.13}$$

So,

$$e^{\tau}_a(x) = x + \tau a(x) + \frac{1}{2}\tau^2 a^2(x) + 0(\tau^3) = {}_2G^{\tau}_{(12\cdots m)}(x) + 0(\tau^3), \quad \tau \sim 0.$$

This shows that ${}_2G^{\tau}_{(12\cdots m)}$ is an approximation, of order 2, to e^{τ}_a. By direct verification it is revertible if each component G^{τ}_i is revertible.

The conclusion (3) is Corollary 4.7 of [6].

Lemma 4 *Given system*

$$\dot{x} = a^{(k)}(x), \quad a^{(k)}(x) = \left(0, \cdots, 0, \frac{\partial b_{k,k+1}}{\partial x_{k+1}}(x), -\frac{\partial b_{k,k+1}}{\partial x_k}(x), 0, \cdots, 0\right)^{\mathrm{T}}, \tag{4.14}$$

with $x = (x_1, \cdots, x_k, x_{k+1}, \cdots, x_n)^{\mathrm{T}}$ *and smooth function* $b_{k,k+1} : \mathbb{R}^n \to \mathbb{R}^n$. *Then any symplectic difference scheme, of order* $p \geq 1$, *of the Hamiltonian system on the* x_k-x_{k+1} *plane*

$$\dot{x}_k = \frac{\partial b_{k,k+1}}{\partial x_{k+1}}, \quad \dot{x}_{k+1} = -\frac{\partial b_{k,k+1}}{\partial x_k} \tag{4.15}$$

with $x_j, j \neq k, k+1$ *as parameters naturally gives a volume-preserving difference scheme, of order* p, *of the source-free system* (4.14) *on the* n*-dimensional* $(x_1, \cdots, x_n)^{\mathrm{T}}$*-space by simply freezing the coordinates* $x_j, j \neq k, k+1$ *and transforming* x_k *and* x_{k+1} *according to the symplectic difference scheme for* (4.15) *in which* $x_j, j \neq k, k+1$ *are considered as frozen parameters.*

Proof. It is obvious that the so-constructed difference scheme is of order p. As to the volume-preserving property, we easily prove that it is true by direct calculation of the determinant of the Jacobian of the step-transition map of the scheme, with the notice of the fact that the determinant of the Jacobian of a symplectic map is equal to one.

Now we construct volume-preserving difference schemes for source-free systems. Let $a = (a_1, \cdots, a_n)^{\mathrm{T}}$ be a source-free field. As was proved in Sect. 3, we have an essentially Hamiltonian decomposition (3.15) for a with the functions $b_{k,k+1}$ given from a by (3.14). We denote by S_k^τ the step-transition map of a volume-preserving difference scheme with step-size τ, as constructed in Lemma 4, associated to the vector field $a^{(k)} = (0, \cdots, 0, \frac{\partial b_{k,k+1}}{\partial x_{k+1}}, -\frac{\partial b_{k,k+1}}{\partial x_k}, 0, \cdots, 0)^{\mathrm{T}}$ for $k = 1, 2, \cdots$. Then by Lemma 3, we have

Theorem 2 *(1) A simple composition of the $n-1$ components $S_1^\tau, S_2^\tau, \cdots, S_{n-1}^\tau$, say*

$$ {}_1G^\tau := S_{n-1}^\tau \circ \cdots \circ S_2^\tau \circ S_1^\tau, \tag{4.16}$$

is a volume-preserving algorithmic approximation, of order one, to e_a^τ; and

$$ {}_2g^\tau := {}_1\hat{G}^{\tau/2} \circ {}_1G^{\tau/2}, \quad {}_2\hat{g}^\tau = {}_1G^{\tau/2} \circ {}_1\hat{G}^{\tau/2} \tag{4.16$'$}$$

are revertible volume-preserving algorithmic approximations, of order 2, to e_a^τ.

(2) If each S_k^τ is an approximation, of order 2, to $e_{a^{(k)}}^\tau$, then the symmetric composition

$$ {}_2G^\tau = S_{n-1}^{\tau/2} \circ \cdots \circ S_2^{\tau/2} \circ S_1^{\tau/2} \circ S_1^{\tau/2} \circ S_2^{\tau/2} \circ \cdots \circ S_{n-1}^{\tau/2} \tag{4.17}$$

is a volume-preserving approximation, of order 2, to e_a^τ.

(3) If each S_k^τ is revertible, then the so-constructed ${}_2G^\tau$ is revertible too.

(4) From the above constructed revertible algorithmic approximation ${}_2g^\tau$ or ${}_2G^\tau$, we can further recursively constructed revertible approximations, of all even orders, to e_a^τ according to the process of Lemma 3.

Remark 1. If a has essentially Hamiltonian decompositions other than (3.15) and (3.14), then one can construct volume-preserving difference schemes corresponding to these decompositions in a similar way to the above.

5 Some special discussions for separable source-free systems

For a source-free field $a = (a_1, \cdots, a_n)^{\mathrm{T}}$ with essentially Hamiltonian decomposition (3.15), we take $S_k^\tau : x = (x_1, \cdots, x_n)^{\mathrm{T}} \to \hat{x} = (\hat{x}_1, \cdots, \hat{x}_n)^{\mathrm{T}}$ as determined from the following

$$\begin{cases} \hat{x}_j = x_j, \quad j \neq k, k+1 \\ \hat{x}_k = x_k + \tau \dfrac{\partial b_{k,k+1}}{\partial x_{k+1}}(x_1, \cdots, x_{k-1}, \hat{x}_k, x_{k+1}, \cdots, x_n) \\ \hat{x}_{k+1} = x_{k+1} - \tau \dfrac{\partial b_{k,k+1}}{\partial x_k}(x_1, \cdots, x_{k-1}, \hat{x}_k, x_{k+1}, \cdots, x_n). \end{cases} \tag{5.1}$$

Then simple calculations show that ${}_1G^\tau = S^\tau_{n-1} \circ \cdots \circ S^\tau_2 \circ S^\tau_1$ is given from

$$
(5.2) \qquad \begin{cases}
\hat{x}_1 = x_1 + \tau a_1(\hat{x}_1, x_2, \cdots, x_n), \\
\hat{x}_j = x_j + \tau a_j(\hat{x}_1, \cdots, \hat{x}_j, x_{j+1}, \cdots, x_n) \\
\qquad\qquad + \tau \int_{x_j}^{\hat{x}_j} \sum_{l=1}^{j-1} \frac{\partial a_l}{\partial x_l}(\hat{x}_1, \cdots, \hat{x}_{j-1}, t, x_{j+1}, \cdots, x_n) dt, \\
\qquad\qquad j = 2, \cdots, n-1, \\
\hat{x}_n = x_n + \tau a_n(\hat{x}_1, \cdots, \hat{x}_{n-1}, x_n)
\end{cases}
$$

and ${}_1\hat{G}^\tau = \left({}_1G^{-\tau}\right)^{-1}$ is given from

$$
(5.3) \qquad \begin{cases}
\hat{x}_n = x_n + \tau a_n(x_1, \cdots, x_{n-1}, \hat{x}_n), \\
\hat{x}_j = x_j + \tau a_j(x_1, \cdots, x_j, \hat{x}_{j+1}, \cdots, \hat{x}_n) \\
\qquad\qquad - \tau \int_{x_j}^{\hat{x}_j} \sum_{l=1}^{j-1} \frac{\partial a_l}{\partial x_l}(x_1, \cdots, x_{j-1}, t, \hat{x}_{j+1}, \cdots, \hat{x}_n) dt, \\
\qquad\qquad j = 2, \cdots, n-1, \\
\hat{x}_1 = x_1 + \tau a_1(x_1, \hat{x}_2, \cdots, \hat{x}_n).
\end{cases}
$$

(5.2) and (5.3) are both volume-preserving difference scheme, of order one, of the source-free system associated to the field a, with the step-transition maps ${}_1G^\tau$ and ${}_1\hat{G}^\tau$. They can be composed into revertible volume-preserving schemes of order 2, say, 2-stage scheme with step transition map ${}_2\hat{g}^\tau = {}_1G^{\tau/2} \circ {}_1\hat{G}^{\tau/2}$: $x = (x_1, \cdots, x_n)^{\mathrm{T}} \to \hat{x} = (\hat{x}_1, \cdots, \hat{x}_n)^{\mathrm{T}}$ as follows

$$
(5.4) \qquad \begin{cases}
\hat{x}_n^{1/2} = x_n + \frac{\tau}{2} a_n(x_1, \cdots, x_{n-1}, \hat{x}_n^{1/2}), \\
\hat{x}_i^{1/2} = x_i + \frac{\tau}{2} a_i(x_1, \cdots, x_i, \hat{x}_{i+1}^{1/2}, \cdots, \hat{x}_n^{1/2}) \\
\qquad\qquad - \frac{\tau}{2} \int_{x_i}^{\hat{x}_i^{1/2}} \sum_{l=1}^{i-1} \frac{\partial a_l}{\partial x_l}(x_1, \cdots, x_{i-1}, t, \hat{x}_{i+1}^{1/2}, \cdots, \hat{x}_n^{1/2}) dt, \\
\qquad\qquad i = 2, \cdots, n-1, \\
\hat{x}_1^{1/2} = x_1 + \frac{\tau}{2} a_1(x_1, \hat{x}_2^{1/2}, \cdots, \hat{x}_n^{1/2}); \\
\hat{x}_1 = \hat{x}_1^{1/2} + \frac{\tau}{2} a_1(\hat{x}_1, \hat{x}_2^{1/2}, \cdots, \hat{x}_n^{1/2}), \\
\hat{x}_j = \hat{x}_j^{1/2} + \frac{\tau}{2} a_j(\hat{x}_1, \cdots, \hat{x}_j, \hat{x}_{j+1}^{1/2}, \cdots, \hat{x}_n^{1/2}) \\
\qquad\qquad + \frac{\tau}{2} \int_{\hat{x}_j^{1/2}}^{\hat{x}_j} \sum_{l=1}^{j-1} \frac{\partial a_l}{\partial x_l}(\hat{x}_1, \cdots, \hat{x}_{j-1}, t, \hat{x}_{j+1}^{1/2}, \cdots, \hat{x}_n^{1/2}) dt, \\
\qquad\qquad j = 2, \cdots, n-1, \\
\hat{x}_n = \hat{x}_n^{1/2} + \frac{\tau}{2} a_n(\hat{x}_1, \cdots, \hat{x}_{n-1}, \hat{x}_n^{1/2}).
\end{cases}
$$

Either (5.2) or (5.3) contains $n-1$ implicit equations generally. But for fields a with some specific properties, it will turn into explicit. For example, if $a = (a_1, \cdots, a_n)^{\mathrm{T}}$ satisfies condition

$$
(5.5) \qquad \frac{\partial a_i}{\partial x_i} = 0, \quad i = 1, \cdots, n
$$

(i.e., a_i does not depend on x_i), then (5.2) turns into

(5.6)
$$\begin{cases} \hat{x}_1 = x_1 + \tau a_1(x_2, \cdots, x_n) \\ \hat{x}_j = x_j + \tau a_j(\hat{x}_1, \cdots, \hat{x}_{j-1}, x_{j+1}, \cdots, x_n), j = 2, \cdots, n-1 \\ \hat{x}_n = x_n + \tau a_n(\hat{x}_1, \cdots, \hat{x}_{n-1}) \end{cases}$$

which is explicit. We note that, for $a = (a_1, \cdots, a_n)^{\mathrm{T}}$,

(5.7)
$$a = \sum_{k=1}^{n} a^{\{k\}}, \quad a^{\{k\}} = (0, \cdots, 0, a_k, 0, \cdots, 0)^{\mathrm{T}}, \quad k = 1, 2, \cdots, n.$$

It is easy to verify that if $a = (a_1, \cdots, a_n)^{\mathrm{T}}$ satisfies the condition (5.5), then the scheme (5.6) is just the result of composing the Euler explicit schemes of the systems associated to the fields $a^{\{k\}}$, $k = 1, \cdots, n$, i.e., we have

(5.8)
$${}_1G^{\tau} = E^{\tau}_{a^{\{n\}}} \circ \cdots \circ E^{\tau}_{a^{\{2\}}} \circ E^{\tau}_{a^{\{1\}}},$$

where

(5.9)
$$E^{\tau}_{a^{\{k\}}} = 1 + \tau a^{\{k\}}, \quad k = 1, 2, \cdots, n, \quad 1 = \text{identity}.$$

In fact, $E^{\tau}_{a^{\{k\}}}$ are the phase flows $e^{\tau}_{a^{\{k\}}}$, since $a^{\{k\}}_* a^{\{k\}} = 0$ for $k = 1, 2, \cdots, n$, which is implied by the condition (5.5). According to Theorem 2, we then get a 2nd order explicit revertible volume-preserving scheme, with step transition map

(5.10)
$$\begin{aligned} {}_2G^{\tau} &= E^{\tau/2}_{a^{\{n\}}} \circ \cdots \circ E^{\tau/2}_{a^{\{2\}}} \circ E^{\tau/2}_{a^{\{1\}}} \circ E^{\tau/2}_{a^{\{1\}}} \circ E^{\tau/2}_{a^{\{2\}}} \circ \cdots \circ E^{\tau/2}_{a^{\{n\}}} \\ &= {}_1G^{\tau/2} \circ {}_1\hat{G}^{\tau/2} = {}_2\hat{g}^{\tau}, \end{aligned}$$

which is given by (5.4) without the integral terms. Also, we can construct explicit revertible volume-preserving schemes of various even orders of the systems of the above type from the ${}_2G^{\tau}$ according to the constructing process stated in Theorem 2.

Systems satisfying the condition (5.5) are important in applications. For example, the well-known ABC flows and Jacobian elliptic curves are described by such systems. From Qin and Zhu's numerical computation for these two examples [7], one may see that volume-preserving algorithms are superior to the non-volume-preserving ones.

In [3,4,15], Feng and Wang introduced the concept of L-separability of vector fields in a Lie subalgebra L of the Lie algebra of all smooth vector fields on $\mathbb{R}^n$ in the sense that the fields can be decomposed as finite sums of vector fields which both belong to L and generate linear phase flows. In this sense, vector fields satisfying the condition (5.5) are source-free separable(all smooth source-free vector fields form a Lie algebra under the usual Lie bracket of vector fields), and so are finite sums of such fields. One easily verifies, in a similar way to that in the Hamiltonian case [3], that all polynomial source-free vector fields are source-free separable. Noting that the above discussions, one can construct explicit revertible volume-preserving difference schemes of various even orders for systems associated to source-free separable vector fields. We call such systems separable source-free ones.

Acknowledgements. The authors would like to thank Qin Meng-zhao, Li Wang-yao, Wang Dao-liu, Zhang Mei-qing, Tang Yi-fa, Zhu Wen-jie, Shu Hai-bing and Jiang Li-xin for their helpful comments.

References

1. Arnold V.I. (1978): Mathematical Methods of Classical Mechanics. Springer, New York
2. Feng Kang (1991): The Hamiltonian way for computing Hamiltonian dynamics, In: R. Spigler, ed., Applied and Industrial Mathematics, p. 17–35, Kluwer, Netherlands
3. Feng Kang, Wang Dao-liu (1991): Variations on a theme by Euler. Preprint, Academia Sinica Computing Center
4. Feng Kang, Wang Dao-liu (1994): Dynamical systems and algorithms for ordinary differential equations. Contemporary Mathematics **163**, 1–32
5. Feng Kang, Wu Hua-mo, Qin Meng-zhao, Wang Dao-liu (1989): Construction of canonical difference schemes for Hamiltonian formalism via generating functions. J. Comp. Math.**7:1**, 71–96
6. Qin Meng-zhao, Zhu Wen-jie (1992): Construction of higher order symplectic schemes by composition. Computing **47**, 309–321
7. Qin Meng-zhao, Zhu Wen-jie (1993): Volume-preserving schemes and numerical experiments. Comp. Math. Appl. **26**, 33–42
8. Shang Zai-jiu (1994): Generating functions for volume-preserving mappings and Hamilton-Jacobi equations for source-free dynamical systems. Science in China (Series A) **37:10**, 1172–1188
9. Shang Zai-jiu (1994): Construction of volume-preserving difference schemes for source-free systems via generating functions. J. Comp. Math. **12:3**, 265–272
10. Spivak M. (1965): Calculus on Manifolds. W. A. Benjamin Inc., New York
11. Strang G. (1968): On the construction and the comparison of difference schemes. SIAM J. Numer. Anal. **12**, 506–517
12. Strang G. (1963): Accurate partial difference methods I: Linear Cauchy problems. Arch. Ration. Mech. Anal. **12**, 392–402
13. Suzuki Masuo (1990): Fractal decomposition of exponential operators with applications to many-body theories and Monte Carlo simulations. Phys. Letters A **146**, 319–323
14. Suzuki Masuo (1992): General theory of higher-order decomposition of exponential operators and symplectic integrators. Phys. Letters A **165**, 387–395
15. Wang Dao-liu (1992): Decomposition of vector fields and composition of algorithms. Feng Kang, Shi Zhong-ci, ed., Proc. Inter. Conf. on Computation of Differential Equations and Dynamical Systems, Beijing, 1992, World Scientific, 1993
16. Warner F.W. (1983): Foundations of Differentiable Manifolds and Lie Groups. Springer, New York
17. Weyl H. (1940): The method of orthogonal projection in potential theory. Duke Math. Journal **7**, 411–444
18. Yoshida H. (1990): Construction of higher order symplectic integrators. Phys. Letters A **150**, 262–268

Note added in the revised version by the second author

This paper represents the result of the close collaboration of the present authors and was written by the second author. The second author must take full responsibility for the mistakes, incompletion of references cited in the manuscript and poor style of this paper. He would like to express his deep sorrow for the death of the first author, suddenly happening on August 17, 1993. Thanks are due to the referees for making some helpful comments and for pointing out the relevant references [11–14] in which the composition difference schemes were already discussed, based on the decompositions of vector fields. The second author also likes to add the references [8] and [9] in which the generating function theory for volume-preserving mappings and Hamilton-Jacobi theory for source-free systems were developed and the volume-preserving difference schemes for source-free systems, based on the generating function method which is different from the method of the present paper, were constructed.

This article was processed by the author using the LaTeX style file *pljour1m* from Springer-Verlag.