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CONSTRUCTION OF VOLUME-PRESERVING DIFFERENCE SCHEMES FOR SOURCE-FREE SYSTEMS VIA GENERETING FUNCTIONS*1)

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1. Introduction

Source-free dynamical systems are of great importance in many branches of physics. A significant subject for such systems is to design "proper" numerical algorithms. Since the phase flows of source-free systems are volume-preserving transformations on the corresponding phase space, the proper way consists in the requirement that the step-transition maps of the algorithms are volume-preserving. We call such algorithms volume-preserving algorithms. In [5], Thyagaraja and Haas designed volume-preserving algorithms for 3-dimensional source-free systems based on a type of generating function representations of volume-preserving mappings on R^3. in [1], Feng Kang and the author gave a more general method to construct volume-preserving difference schemes for general n-dimensional source-free systems based on the decomposition of a source-free vector field on R^n into a sum of $n-1$ essentially 2-dimensional Hamiltonian vector fields and on the well known symplectic difference schemes for 2-dimensional Hamiltonian systems. In this paper, we present another general method for the same purpose whose basis is the generating function apparatus for volume-preserving mappings and Hamilton-Jacobi theory for source-free systems, which have both been well developed by the author[4]. We emphasize that our method presented in this paper provides volume-preserving algorithms for arbitrarily dimensional source-free systems with arbitrarily high order of accuracy which are implicit only in one coordinate and therefore, is superior to the methods given in [5] and in [1] which only provide first order and highly implicit volume-preserving difference schemes respectively.

2. Basic Theorems

The theorems in this section are important to the construction of volume-preserving difference schemes for source-free systems in the next section.

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Theorem 2.1. *Let* $\alpha = \begin{pmatrix} A_\alpha & B_\alpha \\ C_\alpha & D_\alpha \end{pmatrix} \in GL(2n)$. *Denote* $\alpha^{-1} = \begin{pmatrix} A^\alpha & B^\alpha \\ C^\alpha & D^\alpha \end{pmatrix}$. *Let* $g : R^n \to R^n$ *be a differentiable volume-preserving mapping satisfying the transversality condition*

$$\left|C_\alpha \frac{\partial g}{\partial z}(z) + D_\alpha\right| \neq 0 \tag{2.1}$$

in a neighborhood of some $z_0 \in R^n$. *Then there exists a differentiable mapping* $f(w) = f_{\alpha,g} = (f_1(w), f_2(w), \cdots, f_n(w))^T$ *satisfying condition*

$$\left|\frac{\partial f}{\partial w}(w)C_\alpha - A_\alpha\right| = \left|B_\alpha - \frac{\partial f}{\partial w}(w)D_\alpha\right| \neq 0 \tag{2.2}$$

in a neighborhood of the point $w_0 = C_\alpha g(z_0) + D_\alpha z_0$ *in* R^n *such that the mapping* $\hat{z} = g(z)$ *can be reconstructed from* $f = f_{\alpha,g}$ *by the relation*

$$A_\alpha \hat{z} + B_\alpha z = f(C_\alpha \hat{z} + D_\alpha) \tag{2.3}$$

in a neighborhood of the point z_0 *in* R^n. *Conversely, let* $f(w) = (f_1(w), \cdots, f_n(w))^T$ *be a differentiable mapping satisfying condition* (2.2) *in a neighborhood* W *of the point* w_0 *in* R^n. *Then the relation* (2.3) *gives a volume-preserving mapping* $\hat{z} = g(z)$ *satisfying the transversality condition* (2.1) *in a neighborhood of the point* $z_0 = C^\alpha f(w_0) + D^\alpha w_0$ *in* R^n.

Remark 1. Locally speaking, a volume-preserving mapping is completely given from matrix $\alpha \in GL(2n)$ and mapping $f = f_{\alpha,g}$ by the relation (2.3). We call $f = f_{\alpha,g}$ the generating mapping of the type α and the mapping g.

Remark 2. Matrix α represents the type of generating mappings. Specifically we consider some important cases of α. For example, we take

$$\alpha_{(s,s)} = \begin{pmatrix} I_n - E_{ss} & E_{ss} \\ E_{ss} & I_n - E_{ss} \end{pmatrix}, \quad 1 \leq s \leq n, \tag{2.4}$$

where E_{ss} denotes an $n \times n$ matrix of which only entry at the s-th row and s-th column is 1 and all other entries are 0. In this case, equations (2.2) and (2.3) have much more simple forms. For $\alpha = \alpha_{(1,1)}$, for example, (2.2) turns into

$$\frac{\partial f_1}{\partial w_1} = \left|\frac{\partial(f_2, \cdots, f_n)}{\partial(w_2, \cdots, w_n)}\right| \neq 0 \tag{2.5}$$

and (2.3) turns into

$$\begin{cases} z_1 = f_1(\hat{z}_1, z_2, \cdots, z_n), \\ \hat{z}_2 = f_2(\hat{z}_1, z_2, \cdots, z_n), \\ \vdots \\ \hat{z}_n = f_n(\hat{z}_1, z_2, \cdots, z_n). \end{cases} \tag{2.6}$$

For $\alpha_{(s,s)}$, the results are similar.

Remark 3. We note that from (2.5), among the n components of the generating mapping $f(w) = (f_1(w), f_2(w), \cdots, f_n(w))^T$ of the type $\alpha_{(1,1)}$, the last $n-1$ components

$f_2(w), \cdots, f_n(w)$ are independent but required to satisfy the condition

$$\left|\frac{\partial(f_2, \cdots, f_n)}{\partial(w_2, \cdots, w_n)}\right| \neq 0$$

and the first one is determined by these $n-1$ components in the form

$$f_1(w_1, w_2, \cdots, w_n) = c(w_2, \cdots, w_n) + \int_{w_{1,0}}^{w_1} \left|\frac{\partial(f_2, \cdots, f_n)}{\partial(w_2, \cdots, w_n)}\right| (\xi, w_2, \cdots, w_n) d\xi \quad (2.7)$$

for some scalar function $c(w_2, \cdots, w_n)$ depending only on $n-1$ variables.

Theorem 2.2. *Let* $\alpha = \begin{pmatrix} A_\alpha & B_\alpha \\ C_\alpha & D_\alpha \end{pmatrix} \in GL(2n)$. *Denote* $\alpha^{-1} = \begin{pmatrix} A^\alpha & B^\alpha \\ C^\alpha & D^\alpha \end{pmatrix}$. *Suppose* $|C_\alpha + D_\alpha| \neq 0$. *Then there exists a time-dependent generating mapping* $f(w,t) = f_{\alpha,a}(w,t)$ *of the type* α *of the phase flow* g_α^t *of the system*

$$\dot{z} = a(z), a(z) = (a_1(z), \cdots, a_n(z))^T, \quad z = (z_1, \cdots, z_n)^T \quad (2.8)$$

such that

$$\frac{\partial f}{\partial t} = \left(A_\alpha - \frac{\partial f}{\partial w} C_\alpha\right) a(A^\alpha f + B^\alpha w), \quad (2.9)$$

$$f(w, 0) = (A_\alpha + B_\alpha)(C_\alpha + D_\alpha)^{-1} w. \quad (2.10)$$

The proofs of the above two theorems could be found in [4].

(2.9) is the most general Hamilton-Jacobi equations.

Remark 4. If $\alpha = \alpha_{(1,1)}$. Then (2.9) and (2.10) turn into

$$\frac{\partial f_1}{\partial t} = -a_1(w_1, f_2, \cdots, f_n) \frac{\partial f_1}{\partial w_1}, \quad (2.11)_1$$

$$\frac{\partial f_k}{\partial t} = a_k(w_1, f_2, \cdots, f_n) - a_1(w_1, f_2, \cdots, f_n) \frac{\partial f_k}{\partial w_1}, \quad k = 2, \cdots, n, \quad (2.11)_k$$

and

$$f_k(w_1, \cdots, w_n, 0) = w_k, k = 1, 2, \cdots, n, \quad (2.12)_k$$

respectively. If a is source-free, i.e., if

$$\text{div} a(z) = \sum_{k=1}^{n} \frac{\partial a_k}{\partial z_k}(z) = 0, \quad \text{identically in } z \in R^n, \quad (2.13)$$

then g_a^t is volume-preserving. We have

$$\frac{\partial f_1}{\partial w_1}(w,t) = \left|\frac{\partial(f_2, \cdots, f_n)}{\partial(w_2, \cdots, w_n)}\right| (w,t). \quad (2.14)$$

So, from $(2.11)_1$, $(2.12)_1$ and (2.14) we get

$$f_1(w,t) = w_1 - \int_0^t a_1(w_1, f_2(w,\tau), \cdots, f_n(w,\tau)) \left|\frac{\partial(f_2, \cdots, f_n)}{\partial(w_2, \cdots, w_n)}\right| (w,\tau) d\tau. \quad (2.15)$$

$f_2, \cdots, f_n$ are determined independently by $(2.11)_k$ and $(2.12)_k$ for $k = 2, \cdots, n$. We call them the generating functions of the type $\alpha_{(1,1)}$ of the source-free system (2.8).

Theorem 2.3. *Let the vector field $a(z)$ depend analytically on z. Then $f(w,t) = f_{\alpha,a}(w,t)$, the solution of the Cauchy problem (2.9) and (2.10), is expressible as a convergent power series in t for sufficiently small $|t|$, with recursively determined coefficients:*

$$f(w,t) = \sum_{k=0}^{\infty} f^{(k)}(w)t^k, \tag{2.16}$$

$$f^{(0)}(w) = N_0 w, \quad N_0 = (A_\alpha + B_\alpha)(C_\alpha + D_\alpha)^{-1}, \tag*{(2.17)$_0$}$$

$$f^{(1)}(w) = L_0 a(E_0 w), \quad E_0 = (C_\alpha + D_\alpha)^{-1}, \quad L_0 = A_\alpha - N_0 C_\alpha, \tag*{(2.17)$_1$}$$

$k \geq 1$

$$\begin{aligned} f^{(k+1)}(w) = &-\frac{1}{k+1}\frac{\partial f^{(k)}}{\partial w}(w)C_\alpha a(E_0 w) - \frac{1}{k+1}\sum_{m=1}^{k}\sum_{j=1}^{m}\sum_{\substack{i_1+\cdots+i_j=m \\ i_p\geq 1}}\frac{1}{j!} \\ &\times \frac{\partial f^{(k-m)}}{\partial w}(w)C_\alpha D^j_{a,E_0 w}(A^\alpha f^{(i_1)}(w),\cdots,A^\alpha f^{(i_j)}(w)) \\ &+\frac{1}{k+1}\sum_{m=1}^{k}\sum_{\substack{i_1+\cdots+i_m=k \\ i_p\geq 1}}\frac{1}{m!}A_\alpha D^m_{a,E_0 w}(A^\alpha f^{(i_1)}(w),\cdots,A^\alpha f^{(i_m)}(w)) \end{aligned} \tag*{(2.17)$_{k+1}$}$$

where for $\xi^{(k)} = (\xi_1^{(k)},\cdots,\xi_n^{(k)})^T \in R^n, k = 1,2,\cdots,m$,

$$D^m_{a,w}(\xi^{(1)},\cdots,\xi^{(m)}) = \begin{pmatrix} \displaystyle\sum_{\alpha_1,\cdots,\alpha_m=1}^{n} \frac{\partial^m a_1}{\partial z_{\alpha_1}\cdots\partial z_{\alpha_m}}(w)\xi^1_{\alpha_1}\cdots\xi^m_{\alpha_m} \\ \vdots \\ \displaystyle\sum_{\alpha_1,\cdots,\alpha_m=1}^{n} \frac{\partial^m a_n}{\partial z_{\alpha_1}\cdots\partial z_{\alpha_m}}(w)\xi^1_{\alpha_1}\cdots\xi^m_{\alpha_m} \end{pmatrix}. \tag{2.18}$$

Proof. Under our assumption, the generating mapping $f(w,t) = f_{\alpha,a}(w,t)$ depends analytically on w and t in some neighborhood of R^n and for small $|t|$. Expand it as a power series as follows

$$f(w,t) = \sum_{k=0}^{\infty} f^{(k)}(w)t^k.$$

Differentiating it with respect to w and t, we get

$$\frac{\partial f}{\partial w}(w,t) = \sum_{k=0}^{\infty}\frac{\partial f^{(k)}}{\partial w}(w)t^k, \tag{2.19}$$

$$\frac{\partial f}{\partial w}(w,t) = \sum_{k=0}^{\infty}(k+1)f^{(k)}(w)t^k. \tag{2.20}$$

By (2.10),

$$f^{(0)}(w) = f(w,0) = N_0 w,$$

this is $(2.17)_0$. Denote $E_0 = A^\alpha N_0 + B^\alpha = (C_\alpha + D_\alpha)^{-1}$. Then

$$A^\alpha f(w,t) + B^\alpha w = E_0 w + \sum_{k=1}^{\infty} A^\alpha f^{(k)}(w) t^k.$$

Expanding $a(z)$ at $z = E_0 w$, we get

$$\begin{aligned} a(A^\alpha f(w,t) + B^\alpha w) &= a\left(E_0 w + \sum_{k=1}^{\infty} A^\alpha f^{(k)}(w) t^k\right) \\ &= a(E_0 w) + \sum_{k=1}^{\infty} t^k \sum_{m=1}^{k} \sum_{\substack{i_1+\cdots+i_m=k \\ i_p \geq 1}} \frac{1}{m!} D^m_{a,E_0 w}(A^\alpha f^{(i_1)}(w), \cdots, A^\alpha f^{(i_m)}(w)) \end{aligned} \tag{2.21}$$

where D_{a,E_0} is a multilinear operator defined by Eq. (2.18).

Substituting (2.19) and (2.21) into the right hand side of (2.9) and (2.20) into the left hand side of (2.9), then comparing the coefficients of t^k on both sides, we get the recursions $(2.17)_k$. The proof is completed.

Remark 5. $\alpha = \alpha_{(1,1)}$. Then $(2.17)_k$ turn into

$$f^{(0)}(w) = w, \qquad (2.20)_0$$

$$f^{(1)}(w) = \tilde{a}(w), \quad \tilde{a}(w) = (-a_1(w), a_2(w), \cdots a_n(w))^T, \qquad (2.22)_1$$

$k \geq 1$,

$$\begin{aligned} f_i^{(k+1)}(w) = &\frac{1}{k+1} \tilde{a}_1(w) \frac{\partial f_i^{(k)}}{\partial w_1}(w) + \frac{1}{k+1} \sum_{m=1}^{k-1} \sum_{j=1}^{m} \sum_{\substack{i_1+\cdots+i_j=m \\ i_p \geq 1}} \sum_{\alpha_1,\cdots,\alpha_j=2}^{n} \frac{1}{j!} \\ &\times \frac{\partial f_i^{(k-m)}}{\partial w_1}(w) \frac{\partial^j \tilde{a}_1}{\partial w_{\alpha_1} \cdots \partial w_{\alpha_j}}(w) f_{\alpha_1}^{(i_1)}(w) \cdots f_{\alpha_j}^{(i_j)}(w) \\ &+ \frac{1}{k+1} \sum_{m=1}^{k} \sum_{\substack{i_1+\cdots+i_m=k \\ i_p \geq 1}} \sum_{\alpha_1,\cdots,\alpha_m=2}^{n} \frac{1}{m!} \\ &\times \frac{\partial^m \tilde{a}_i}{\partial w_{\alpha_1} \cdots \partial w_{\alpha_m}}(w) f_{\alpha_1}^{(i_1)}(w) \cdots f_{\alpha_m}^{(i_m)}(w), \quad i = 1, 2, \cdots, n. \end{aligned} \qquad (2.22)_{k+1}$$

3. Construction of Volume-Preserving Difference Schemes

In this section, we consider the construction of volume-preserving difference schemes for the source-free system (2.8). By Remark 2 of Theorem 2.1, for given time-dependent scalar functions $\phi_2(w,t), \cdots, \phi_n(w,t) : R^n \times R \to R$ and $c(\tilde{w},t) : R^{n-1} \times R \to R$, we can get a time-dependent volume-preserving mapping $\tilde{g}(z,t)$. If $\phi_2(w,t), \cdots, \phi_n(w,t)$ approximate the generating functions $f_2(w,t), \cdots, f_n(w,t)$ of the type $\alpha_{(1,1)}$ of the source-free system (2.8), then for a suitable choice of $c(\tilde{w},t), \tilde{g}(w,t)$ approximates the phase flow $g^t_\alpha(z) = g(z,t)$. Fixing t as a time step, we can get a difference scheme—volume-preserving difference scheme—whose transition from one time-step to the next is volume-preserving. By Remark 5 of Theorem 2.3 generating functions $f_2(w,t),\cdots,f_n(w,t)$ can be expressed as power series. So a natural way to approximate $f_2(w,t),\cdots,f_n(w,t)$ is to take the truncations of the series. However, we have to choose a suitable $c(\tilde{w},t)$ in (2.7) in order to guarantee the accuracy of the scheme.

Assume that

$$\phi_i^{(m)}(w,t) = \sum_{k=0}^{m} f_i^{(k)}(w)t^k, \quad i = 2,\cdots,n \tag{3.1}$$

and

$$\psi_1^{(m)}(w,t) = \sum_{k=0}^{m} f_1^{(k)}(w)t^k. \tag{3.2}$$

Let, for some fixed value $w_{1,0}$,

$$c^{(m)}(w_2,\cdots,w_n,t) = \psi_1^{(m)}(w_{1,0},w_2,\cdots,w_n,t) \tag{3.3}$$

and

$$\phi_1^{(m)}(w,t) = c^{(m)}(w_2,\cdots,w_n,t) + \int_{w_{1,0}}^{w_1} \left|\frac{\partial(\phi_2^{(m)},\cdots,\phi_n^{(m)})}{\partial(w_2,\cdots,w_n)}\right|(\xi,w_2,\cdots,w_n,t)d\xi. \tag{3.4}$$

Then we have

Theorem 3.1. *Using Theorems 2.2 and 2.3, for sufficiently small $\tau \geq 0$ as the time-step, define mapping $\phi^{(m)}(w,\tau) = (\phi_1^{(m)}(w,\tau),\phi_2^{(m)}(w,\tau),\cdots,\phi_n^{(m)}(w,\tau))^T$ with the components $\phi_i^{(m)}(w,\tau), i = 1,2,\cdots,n$ given as above for $m = 1,2,\cdots$, then the mapping*

$$w \to \hat{w} = \phi^{(m)}(w,\tau) \tag{3.5}$$

defines a volume-preserving difference scheme $z = z^k \to z^{k+1} = \hat{z}$,

$$\begin{cases} z_1^k = \phi_1^{(m)}(z_1^{k+1},z_2^k,\cdots,z_n^k,\tau), \\ \hat{z}_i^{k+1} = \phi_i^{(m)}(z_1^{k+1},z_2^k,\cdots,z_n^k,\tau), \end{cases} \quad i = 2,\cdots,n \tag{3.6}$$

of m-th order of accuracy of the source-free system (2.8).

Proof. Since $\phi_i^{(m)}(w,0) = f_i^{(0)}(w,0) = w_i, i = 2,\cdots,n$,

$$\left|\frac{\partial(\phi_2^{(m)},\cdots,\phi_n^{(m)})}{\partial(w_2,\cdots,w_n)}\right|(w,0) = 1.$$

Therefore, for sufficiently small τ and in some neighborhood of R^n,

$$\left|\frac{\partial(\phi_2^{(m)},\cdots,\phi_n^{(m)})}{\partial(w_2,\cdots,w_n)}\right|(w,\tau) \neq 0.$$

By Theorem 2.1, Remark 2, Remark 3 and Eq. (3.4), the relation (3.6) defines a time-dependent volume-preserving mapping $z = z^k \to z^{k+1} = \hat{z} = \tilde{g}(z,\tau)$. That is, (3.6) is a volume-preserving difference scheme.

Noting that

$$\phi_i^{(m)}(w,\tau) = f_i(w,\tau) + O(\tau^{m+1}), \quad i = 2,\cdots,n,$$
$$\psi_1^{(m)}(w,\tau) == f_1(w,\tau) + O(\tau^{m+1})$$

for sufficiently small τ, and

$$f_1(w,\tau) = f_1(w_{1,0}, w_2, \cdots, w_n, \tau) + \int_{w_{1,0}}^{w_1} \left| \frac{\partial(f_2,\cdots,f_n)}{\partial(w_2,\cdots,w_n)} \right| (\xi, w_2, \cdots, w_n) d\xi,$$

we have from (3.4)

$$\phi_1^{(m)}(w,\tau) = f_1(w,\tau) + O(\tau^{m+1}).$$

So, $\phi^{(m)}(w,\tau) = (\phi_1^{(m)}(w,\tau), \phi_2^{(m)}(w,\tau), \cdots, \phi_n^{(m)}(w,\tau))^T$ is an m-th order approximant to $f(w,\tau) = (f_1(w,\tau), f_2(w,\tau), \cdots, f_n(w,\tau))^T$, the generating mapping of the type $\alpha_{(1,1)}$ of g_a^t and hence the volume-preserving difference scheme (3.6) is of m-th order of accuracy. The proof is completed.

Remark 6. We note that the volume-preserving difference scheme $z^k \to z^{k+1}$ given by (3.6) is implicit for only one new variable z_1^{k+1} and explicit for all other new variables $z_i^{k+1}, i = 2, \cdots, n$ in terms of the old variables $z_i^k, i = 1, 2, \cdots, n$.

Remark 7. We can get volume-preserving difference schemes similar to the above one if we consider the types $\alpha = \alpha_{(s,s)}$ for $2 \le s \le n$ instead of $\alpha = \alpha_{(1,1)}$.

As examples, next we give first order and second order volume-preserving difference schemes. Without loss of the generality, we take $w_{1,0} = 0$.

1° First order scheme

$$\begin{cases} z_1^k = \phi_1^{(1)}(z_1^{k+1}, z_2^k, \cdots, z_n^k, \tau), \\ z_i^{k+1} = \phi_i^{(1)}(z_1^{k+1}, z_2^k, \cdots, z_n^k, \tau), \end{cases} \quad i = 2, \cdots, n,$$

where

$$\phi_1^{(1)}(w,\tau) = -\tau a_1(0, w_2, \cdots, w_n)$$
$$+ \int_0^{w_1} \begin{vmatrix} 1 + \tau\frac{\partial a_2}{\partial w_2} & \tau\frac{\partial a_2}{\partial w_3} & \cdots & \tau\frac{\partial a_2}{\partial w_n} \\ \tau\frac{\partial a_3}{\partial w_2} & 1 + \tau\frac{\partial a_3}{\partial w_3} & \cdots & \tau\frac{\partial a_3}{\partial w_n} \\ \cdots & \cdots & \cdots & \cdots \\ \tau\frac{\partial a_n}{\partial w_2} & \tau\frac{\partial a_n}{\partial w_3} & \cdots & 1 + \tau\frac{\partial a_n}{\partial w_n} \end{vmatrix} (\xi, w_2, \cdots, w_n) d\xi,$$

$$\phi_i^{(1)}(w,\tau) = w_i + \tau a_i(w).$$

2° Second order scheme

$$\begin{cases} z_1^k = \phi_1^{(2)}(z_1^{k+1}, z_2^k, \cdots, z_n^k, \tau), \\ z_i^{k+1} = \phi_i^{(2)}(z_1^{k+1}, z_2^k, \cdots, z_n^k, \tau), \end{cases} \quad i = 2, \cdots, n$$

where

$$\phi_1^{(2)}(w,\tau) = \psi_1^{(2)}(0,w_2,\cdots,w_n,\tau) + \int_0^{w_1} \left|\frac{\partial\psi_2^{(2)},\cdots\psi_n^{(2)}}{\partial(w_2,\cdots,w_n)}\right| (\xi,w_2,\cdots,w_n)d\xi,$$

$$\phi_i^{(2)}(w,\tau) = \psi_i^{(2)}(w,\tau), \quad i=2,\cdots,n,$$

and

$$\psi^{(2)}(w,\tau) = (\psi_1^{(2)}(w,\tau),\cdots,\psi_n^{(2)}(w,\tau))^T = w + \tau\tilde{a}(w) + \frac{1}{2}\tau^2\frac{\partial\tilde{a}}{\partial w}(w)\tilde{a}(w),$$

$$\tilde{a}(w) = (-a_1(w), a_2(w),\cdots,a_n(w))^T.$$

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