DISCRETE AND CONTINUOUS
DYNAMICAL SYSTEMS
Volume **34**, Number **3**, March **2014**

doi:10.3934/dcds.2014.34.1229

pp. **1229–1249**

GENERATING FUNCTIONS AND VOLUME PRESERVING MAPPINGS

Huiyan Xue[1] and Antonella Zanna

Department of Mathematics, University of Bergen
P.O. Box 7800, N-5020 Bergen, Norway

Dedicated to Arieh Iserles: A wise mentor, brilliant colleague and wonderful friend

Abstract. In this paper, we study generating forms and generating functions for volume preserving mappings in $\mathbf{R}^n$. We derive some parametric classes of volume preserving numerical schemes for divergence free vector fields. In passing, by extension of the Poincaré generating function and a change of variables, we obtained symplectic equivalent of the theta-method for differential equations, which includes the implicit midpoint rule and symplectic Euler A and B methods as special cases.

1. **Introduction.** Generating functions have been known for a long time in the context of symplectic integration. These functions possess many nice properties: they describe entirely the dynamics of mechanical systems, they are smooth solutions of the Hamilton-Jacobi differential equations, they are directly connected to any symplectic map (see for instance [1, 13], and the more numerically oriented [15, 10, 8]).

The scope of this paper is a study of the method of generating functions (and forms) to preserve canonical volume forms by numerical integrators. Because of *no-go* theorems [3, 9], it is not possible to construct volume preserving methods for generic divergence free vector fields within the class of B-series methods. B-series methods include all classical integrators like Taylor-expansion based methods, Runge–Kutta methods and multistep methods. Splitting methods do not fall in the class of B-series methods and several methods based on such approach have been proposed, see for instance [12], the more recent [22], and references therein. Generating functions and generating forms have the property that they include B-series type methods as well as splitting methods as particular cases. It is therefore reasonable that such approach can be used to obtain new numerical methods that preserve volume.

Differently from the symplectic case, the generating function (and generating form) approach for volume forms is not well understood. Some earlier works on this topic are [17, 18], extending the Hamiltonian technique of [4, 7], that used linear

2010 *Mathematics Subject Classification.* Primary: 53D22, 70H15; Secondary: 65L05.
Key words and phrases. Generating function, symplectic, volume preserving, differential forms.
This work was support by NFR grant Geometric Numeric Integration in Applications, project no. 191178/V30 and by a Marie Curie International Research Staff Exchange Scheme Fellowship (CRISP) within the 7th European Community Framework Programme.
[1]Corresponding author

maps in the product space, to volume preserving forms, thus obtaining an equivalent of the Hamilton-Jacobi differential equation [18]. To obtain a first and second order scheme, Shang imposed simplifying conditions, requiring the transformation matrix to be a special case of Hadamard matrix. More recent work on the topic, though from a different perspective, is by Carroll [2] who gave the representation for the n dimensional volume preserving transformations by $n-1$ potential functions. In [11], Lomeli and Meiss studied exact volume preserving mappings and gave thirty-six generating forms on $\mathbf{R}^3$. The latter paper paves the background for our investigations.

The paper is organized as follows. We will present some background and notation on volume preservation and generating functions (resp. forms) in Section 1. In Section 2, we discuss the volume preserving generating form approach of [2, 11]. The generating forms are associated to *generic* volume preserving maps and there is a-priori no immediate connection between them and the vector field of a given divergence free differential equation. Our contribution is to identify a class of primitive forms which we can directly associate to a given vector field. This class of primitives corresponds to a splitting in two-dimensional Hamiltonian systems, treated by symplectic Euler schemes, thus recovering a volume preserving splitting method originally proposed by Feng and Shang [5].

In Section 3, we recall the definition of the Poincaré's generating function [19]. By using a linear change of variables, we generalise the approach to obtain a one-parameter-family of methods, the symplectic ϑ-methods. A similar change of variables is used to obtain some new classes of generating forms for the volume preserving case. Lastly, we give some conclusions and future plans in Section 4.

1.1. **Background and notation.** We study ordinary differential equations of the form

$$\dot{\mathbf{x}} = \mathbf{a}(\mathbf{x}), \quad \mathbf{x}(0) = \mathbf{x}_0, \tag{1}$$

where $\mathbf{x} \in \mathbf{R}^n$ and $\mathbf{a} : \mathbf{R}^n \to \mathbf{R}^n$, $\mathbf{a}(\mathbf{x}) = [a_1(\mathbf{x}), \ldots, a_n(\mathbf{x})]^T$, is subject to the divergence free condition

$$\nabla \cdot \mathbf{a} = \sum_{i=1}^{n} \partial_{x_i} a_i(\mathbf{x}) = 0. \tag{2}$$

It is well known that divergence free equations preserve volume (see for instance [8]), and it is our interest to study numerical methods (maps $\mathbf{x} \mapsto \mathbf{X}$) that share the same property.

Recall that a volume form Ω on a n-dimensional manifold $\mathcal{M}$ is a fully skew-symmetric, non-degenerate, n-form. For convenience, we have collected some basic definitions and properties of differential forms and differential calculus in Appendix A.

Definition 1.1. (*Volume preservation*). A volume form Ω on a manifold $\mathcal{M}$ is preserved by a diffeomorphism $\mathbf{f} : \mathcal{M} \mapsto \mathcal{M}$ if

$$\mathbf{f}^*\Omega = \Omega, \tag{3}$$

where $\mathbf{f}^*$ denotes the pullback of $\mathbf{f}$. Such a map $\mathbf{f}$ is called a *canonical transformation.*

Assume $\mathcal{M} = \mathbf{R}^n$, and consider the canonical coordinates $x_1, x_2, \ldots, x_n$ and the canonical volume form $\Omega = dx_1 \wedge dx_2 \wedge \cdots \wedge dx_n$. For any n vectors, $\mathbf{v}_1, \ldots, \mathbf{v}_n$,

$\Omega(\mathbf{v}_1,\ldots,\mathbf{v}_n) = dx_1\wedge\cdots\wedge dx_n(\mathbf{v}_1,\ldots,\mathbf{v}_n) = \det[\mathbf{v}_1,\ldots,\mathbf{v}_n]$. The volume preservation condition (3) for the map $\mathbf{f} : (x_1, x_2,\ldots,x_n) \mapsto (X_1, X_2,\ldots,X_n)$, becomes

$$dX_1 \wedge dX_2 \wedge\cdots\wedge dX_n = dx_1 \wedge dx_2 \wedge\cdots\wedge dx_n, \tag{4}$$

and it is equivalent to requiring that $\mathbf{f}$ has unit Jacobian determinant,

$$\left|\frac{\partial(X_1, X_2,\ldots,X_n)}{\partial(x_1, x_2,\ldots,x_n)}\right| = 1, \tag{5}$$

as the vectors $\mathbf{v}_1,\ldots,\mathbf{v}_n$ are transported by the linearization (Jacobian matrix) of $\mathbf{f}$. Thus volume preserving maps can be constructed either using the algebraic rules of the differential forms (4) or directly using the Jacobian determinant condition (5). In this paper we will address the problem using differential forms.

A special case of volume preservation is the symplectic case. Consider the column vectors $\mathbf{p} = [p_1, p_2,\ldots,p_d]^T$ and $\mathbf{q} = [q_1, q_2,\ldots,q_d]^T$. The map $\mathbf{f} : (\mathbf{p},\mathbf{q}) \mapsto (\mathbf{P},\mathbf{Q})$ is *symplectic* if

$$d\mathbf{P} \wedge d\mathbf{Q} = d\mathbf{p} \wedge d\mathbf{q}. \tag{6}$$

i.e. $\mathbf{f}$ preserves the canonical two-form $\omega = d\mathbf{p}\wedge d\mathbf{q}$. If ω is an arbitrary symplectic form (not necessarily canonical), then the symplecticness condition of the map $\mathbf{f}$ is similar to (3), namely, $\mathbf{f}^*\omega = \omega$.

When ω is exact ($\omega = d\nu$), a map $\mathbf{f} : (\mathbf{p},\mathbf{q}) \mapsto (\mathbf{P},\mathbf{Q})$ obeying (6) is an *exact symplectic map*. Thus, assume $\omega = d\nu$, where ν is a one-form. We obtain $\mathbf{f}^*d\nu - d\nu = 0$, from which $d(\mathbf{f}^*\nu - \nu) = 0$, that is,

$$\mathbf{f}^*\nu - \nu = dS, \tag{7}$$

The 0-form (function) S is called a *generating function*. For instance, the one form $\nu = \mathbf{p}^T d\mathbf{q}$, which is obviously a primitive of ω, one has

$$\mathbf{P}^T d\mathbf{Q} - \mathbf{p}^T d\mathbf{q} = dS, \tag{8}$$

where $S = S(\mathbf{q},\mathbf{Q})$.

A similar procedure can be extended to the volume form case.

Definition 1.2. [11]. Let Ω be a volume form and ν a primitive, i.e. $\Omega = d\nu$. A diffeomorphism $\mathbf{f} : \mathbf{R}^n \mapsto \mathbf{R}^n$ is ν-exact volume preserving if there exists a $n-2$ form λ on $\mathbf{R}^n$ such that

$$\mathbf{f}^*\nu - \nu = d\lambda. \tag{9}$$

Primitives ν of a differential n-form are not uniquely determined. This motivates the generalization below.

Definition 1.3. [11]. Suppose that $d\nu = d\tilde{\nu} = \Omega$ (volume form). A diffeomorphsim $\mathbf{f} : \mathbf{R}^n \mapsto \mathbf{R}^n$ is exact volume preserving with respect to $(\nu, \tilde{\nu})$ if

$$\mathbf{f}^*\tilde{\nu} - \nu = d\lambda, \tag{10}$$

for a $n-2$ form λ. λ is called a *generating form*.

For the symplectic case, there are two primitives to consider (up to the d- of a scalar function), $\mathbf{p}^T d\mathbf{q}$ and $-\mathbf{q}^T d\mathbf{p}$. Thus, all possible cases can be summarized in a table, see Table 1.

Remark 1. Our ultimate goal is to devise numerical methods where $\mathbf{P} = \mathbf{P}(\Delta t) \to \mathbf{p}$ and $\mathbf{Q} = \mathbf{Q}(\Delta t) \to \mathbf{q}$ as $\Delta t \to 0$, namely maps that are consistent with the identity map. Note that the generating functions of type I. and IV., Table 1, are not consistent with the identity map. For instance, for case I., which is described

$\mathbf{f}^*\tilde{\nu}\downarrow \quad \nu\rightarrow$	$\mathbf{p}^T d\mathbf{q}$	$-\mathbf{q}^T d\mathbf{p}$
$\mathbf{P}^T d\mathbf{Q}$	I. $S(\mathbf{q},\mathbf{Q})$ $\mathbf{P}=\partial_{\mathbf{Q}}S(\mathbf{q},\mathbf{Q})$ $\mathbf{p}=-\partial_{\mathbf{q}}S(\mathbf{q},\mathbf{Q})$ $\frac{\partial\mathbf{p}}{\partial\mathbf{Q}}\neq 0$	II. $S(\mathbf{p},\mathbf{Q})$ $\mathbf{P}=\partial_{\mathbf{Q}}S(\mathbf{p},\mathbf{Q})$ $\mathbf{q}=\partial_{\mathbf{p}}S(\mathbf{p},\mathbf{Q})$ $\frac{\partial\mathbf{q}}{\partial\mathbf{Q}}\neq 0$
$-\mathbf{Q}^T d\mathbf{P}$	III. $S(\mathbf{q},\mathbf{P})$ $\mathbf{Q}=\partial_{\mathbf{P}}S(\mathbf{q},\mathbf{P})$ $\mathbf{p}=\partial_{\mathbf{q}}S(\mathbf{q},\mathbf{P})$ $\frac{\partial\mathbf{p}}{\partial\mathbf{P}}\neq 0$	IV. $S(\mathbf{p},\mathbf{P})$ $\mathbf{Q}=\partial_{\mathbf{P}}S(\mathbf{p},\mathbf{P})$ $\mathbf{q}=-\partial_{\mathbf{p}}S(\mathbf{p},\mathbf{P})$ $\frac{\partial\mathbf{q}}{\partial\mathbf{P}}\neq 0$

TABLE 1. The four classical types of generating functions for the canonical symplectic form $\omega = d\mathbf{p}\wedge d\mathbf{q}$.

by (8), the determining equations for $\mathbf{p}$ and $\mathbf{P}$ do not yield in the limit, since $d\mathbf{q}$ and $d\mathbf{Q}$ are not independent. Nevertheless, they can be used to obtain symplectic numerical methods, which, however, are singular in the limit. Such generating functions have been used, among others, by [1, 14] and in the context of discrete Lagrangian methods, see [10]. In this paper, however, we will focus only on maps that are compatible with the identity.

In the volume case, one can generate similar tables, starting from $\nu = (-1)^{n-1}\cdot x_n dx_1\wedge dx_2\wedge\cdots\wedge dx_{n-1}$, and taking $\tilde{\nu}$ as ν with permutation of the variables. Differently from the symplectic case, which is characterized by a single scalar function for any of the cases in Table 1, the n-dimensional volume preserving case is determined by $n-1$ functions: for instance, f_i can be determined by other functions $f_1,\ldots,f_{i-1},f_{i+1},\ldots,f_n$ due to (5). There are several ways to choose the independent functions and they are related to the coefficient functions of the $n-2$ forms λ. The $n=3$ case is described at length in [11]: for a fixed choice of ν and $\tilde{\nu}$, the 1-form λ is written as the sum of two 1-forms in four essentially different ways. For each of the two 1-forms, a coefficient function (the analogous of S in the symplectic case) is needed. In other words, the two coefficient functions of λ can be systematically chosen out of a set of functions, A,B,C,D, in four different ways. As there are three possible choices of ν and $\tilde{\nu}$ (giving nine choices of $(\nu,\tilde{\nu})$), this gives a total of 36 possible generating forms just for the $n=3$ case. Fortunately, it suffices to tabulate the four choices of the 1-form λ when $\nu=\tilde{\nu}=x_3dx_1\wedge dx_2$ (corresponding to case I. in the symplectic setting). All the other cases can be obtained from this basic table by applying a permutation of the indices to the lowercase and uppercase variables.

In the symplectic case, the generating function S is related to the Hamiltonian H of the system, either directly (for instance, $S=\mathbf{Q}^T\mathbf{p}-\Delta t H(\mathbf{Q},\mathbf{p})$ in case II., yielding a first order symplectic Euler method), or implicitly through Legendre transforms as in case I. [13, 10], see Table 1. This relation between the generating function and the Hamiltonian function can then be used to obtain numerical methods for a given Hamiltonian vector field. From Table 2, one realises that there is no immediate connection between the components $a_i(\mathbf{x})$ of the vector field (1) and the functions A,B,C,D even in the case $n=3$. Our goal is to identify generating forms that can be associated systematically to the components of a vector field, so to obtain a numerical method, as in the Hamiltonian setting.

(123,123)	Adx_1	Bdx_2
CdX_1	$\lambda = A(x_1,x_2,X_1)dx_1 + C(x_1,X_1,X_2)dX_1$ $x_3 = \partial_{x_2}A$ $\partial_{X_1}A = \partial_{x_1}C$ $X_3 = -\partial_{X_2}C$ $\frac{\partial X_1}{\partial x_3} \neq 0, \quad \frac{\partial x_1}{\partial X_3} \neq 0$	$\lambda = B(x_1,x_2,X_1)dx_2 + C(x_2,X_1,X_2)dX_1$ $x_3 = -\partial_{x_1}B$ $\partial_{X_1}B = \partial_{x_2}C$ $X_3 = -\partial_{X_2}C$ $\frac{\partial X_1}{\partial x_3} \neq 0, \quad \frac{\partial x_2}{\partial X_3} \neq 0$
DdX_2	$\lambda = A(x_1,x_2,X_2)dx_1 + D(x_1,X_1,X_2)dX_2$ $x_3 = \partial_{x_2}A$ $\partial_{X_2}A = \partial_{x_1}D$ $X_3 = \partial_{X_1}D$ $\frac{\partial X_2}{\partial x_3} \neq 0, \quad \frac{\partial x_1}{\partial X_3} \neq 0$	$\lambda = B(x_1,x_2,X_2)dx_2 + D(x_2,X_1,X_2)dX_2$ $x_3 = -\partial_{x_1}B$ $\partial_{X_2}B = \partial_{x_2}D$ $X_3 = \partial_{X_1}D$ $\frac{\partial X_2}{\partial x_3} \neq 0, \quad \frac{\partial x_2}{\partial X_3} \neq 0$

TABLE 2. The four basic types of generating 1-forms λ for $\nu = \tilde{\nu} = x_3 dx_1 \wedge dx_2$, adapted from [11]. These forms are the volume preserving "equivalent" of the generating functions of type I. for the symplectic case. All the other tables are obtained by applying cyclic permutations to the variables (x_1,x_2,x_3) and (X_1,X_2,X_3).

Our findings in Section 2 can be summarised as follows. The type II. and III. generating functions of the symplectic case correspond to the case $\tilde{\nu} \neq \nu$. For $n = 3$, these (6 tables, 24 cases) are be obtained from Table 2 by applying a permutation of the indices:

$$\begin{array}{ll} (123,231), & (231,123), \\ (123,312), & (312,123), \\ (231,312), & (312,231), \end{array} \tag{11}$$

where the first term in each ordered couple corresponds to the corresponding permutation of the $\mathbf{x}$ variables and the second permutation refers to the $\mathbf{X}$. For instance, $(312,231)$ means that $(x_1,x_2,x_3) \mapsto (x_3,x_1,x_2)$ and $(X_1,X_2,X_3) \mapsto (X_2,X_3,X_1)$. For each such table, containing four possible generating 1-forms, we identify the unique 1-form having the property $\frac{\partial X_i}{\partial x_i} \neq 0$, $\frac{\partial x_j}{\partial X_j} \neq 0$ for two of the indices $i,j \in \{1,2,3\}$. It is exactly these 1-forms we solve for and associate to a divergence free vector field in a suitable representation.

Out of these six cases associated to the permutations in (11), we recognise that those in the left column of (11) correspond to different normalisations of the divergence free vector field:

$$\begin{aligned} \dot{x}_1 &= \frac{\partial F^{(1)}}{\partial x_2} \\ \dot{x}_2 &= -\frac{\partial F^{(1)}}{\partial x_1} + \frac{\partial F^{(2)}}{\partial x_3} \\ \dot{x}_3 &= -\frac{\partial F^{(2)}}{\partial x_2} \end{aligned}$$

$(123,\ 231)$, A-D

$$\begin{aligned} \dot{x}_1 &= -\frac{\partial F^{(1)}}{\partial x_2} + \frac{\partial F^{(2)}}{\partial x_3} \\ \dot{x}_2 &= \frac{\partial F^{(1)}}{\partial x_1} \\ \dot{x}_3 &= -\frac{\partial F^{(2)}}{\partial x_1} \end{aligned}$$

$(123,\ 312)$ B-C

$$\begin{aligned} \dot{x}_1 &= \frac{\partial F^{(1)}}{\partial x_3} \\ \dot{x}_2 &= -\frac{\partial F^{(2)}}{\partial x_3} \\ \dot{x}_3 &= -\frac{\partial F^{(1)}}{\partial x_1} + \frac{\partial F^{(2)}}{\partial x_2} \end{aligned}$$

$(231,\ 312)$ A-D

Concerning the cases listed in the second column of (11), note that the role of the lower case and upper case variables is interchanged. In the context of numerical integrators, they correspond to the *adjoint* numerical methods. For instance, $(231, 123)$ will generate the adjoint method of $(123, 231)$, under the appropriate normalization of the vector field.

2. Volume-preserving mappings by the generating functions (resp. forms) approach.

2.1. Carroll's generating function.

For $n = 3$, Carroll [2] studied the transformation

$$\begin{aligned} X_1 &= f_1(x_1, x_2, x_3), \\ X_2 &= f_2(x_1, x_2, x_3), \\ X_3 &= f_3(x_1, x_2, x_3), \end{aligned}$$

subject to the volume preserving condition (5),

$$\left| \frac{\partial(x_1, x_2, x_3)}{\partial(X_1, X_2, X_3)} \right| = 1. \tag{12}$$

To solve (12), Carroll introduced the intermediate variables $(x_1^{'}, x_2^{'}, x_3^{'})$,

$$x_1 = x_1^{'},\ x_2 = x_2^{'},\ x_3 = h(x_1^{'}, x_2^{'}, x_3^{'}), \tag{13}$$

and a 'pseudo-planar' deformation

$$X_1 = g_1(x_1^{'}, x_2^{'}, x_3^{'}),\ X_2 = g_2(x_1^{'}, x_2^{'}, x_3^{'}),\ X_3 = x_3^{'}. \tag{14}$$

The Jacobian satisfies

$$\left| \frac{\partial(X_1, X_2, X_3)}{\partial(x_1^{'}, x_2^{'}, x_3^{'})} \right| = \left| \frac{\partial(x_1^{'}, x_2^{'}, x_3^{'})}{\partial(x_1, x_2, x_3)} \right|. \tag{15}$$

Substituting (13) and (14) into (15) gives

$$\left| \frac{\partial(g_1, g_2)}{\partial(x_1, x_2)} \right| = \left| \frac{\partial h}{\partial X_3} \right|, \tag{16}$$

which implies $x_3 = h(x_1, x_2, X_3)$. Introducing a potential function $\Phi(x_1, X_2, X_3)$, it is showed that the solution of (16) is given as

$$X_1 = \frac{\partial}{\partial X_2}\Phi(x_1, X_2, X_3),\ \int \frac{\partial}{\partial X_3} h(x_1, x_2, X_3) = \frac{\partial}{\partial x_1}\Phi(x_1, X_2, X_3).$$

Equations (13) and (14) imply

$$x_3 = h(x_1, x_2, X_3).$$

By introducing another potential function $\Psi(x_1, x_2, X_3)$ and setting $h(x_1, x_2, X_3) = \frac{\partial}{\partial x_2}\Psi(x_1, x_2, X_3)$, the general solution now takes the form

$$\begin{aligned} X_1 &= \frac{\partial}{\partial X_2}\Phi(x_1, X_2, X_3), \\ \frac{\partial}{\partial x_1}\Phi(x_1, X_2, x_3) &= \frac{\partial}{\partial X_3}\Psi(x_1, x_2, X_3), \\ x_3 &= \frac{\partial}{\partial x_2}\Psi(x_1, x_2, X_3), \end{aligned} \tag{17}$$

under the *twist conditions*

$$\frac{\partial^2}{\partial x_1 \partial X_2}\Phi(x_1, X_2, X_3) \neq 0, \qquad \frac{\partial^2}{\partial x_2 \partial X_3}\Psi(x_1, x_2, X_3) \neq 0, \tag{18}$$

which are necessary in order to solve the second equation of (17).

Remark 2. Note that the conditions (17)-(18) are precisely those in the A-D case in Table 2 for the permutation $(123, 231)$.

Remark 3. For the choice $\Phi = x_1X_2$ and $\Psi = x_2X_3$, the generating function approach generates the identity map. This property is crucial since we are interested in obtaining numerical schemes for the differential equations, with consistence properties in the limit when $\mathbf{X} \to \mathbf{x}$, see also Remark 1.

The approach can be generalized to $\mathbf{R}^n$ as follows.

Theorem 2.1. [11]. *Let $\Phi^{(1)}, \dots, \Phi^{(n-1)}$ be C^2 functions on $\mathbf{R}^n$. If the conditions*

$$\frac{\partial^2}{\partial x_r \partial X_{r+1}}\Phi^{(r)}(x_1, \dots, x_r, X_{r+1}, \dots, X_n) \neq 0, \quad r = 1, \dots, n-1,$$

are satisfied, the $n-2$ generating form

$$\lambda = \sum_{k=1}^{n} \Phi^{(k)} dx_1 \wedge \cdots \wedge dx_{k-1} \wedge dX_{k+2} \wedge \cdots \wedge dX_n \tag{19}$$

generates a canonical map $(X_1, \dots, X_n) = \mathbf{f}(x_1, \dots, x_n)$ implicitly given by the n equations

$$X_1 = \partial_{X_2}\Phi^{(1)}(x_1, X_2, \dots, X_n), \tag{20}$$

$$\partial_{x_k}\Phi^{(k)}(x_1, \dots, x_k, X_{k+1}, \dots, X_n) = \partial_{X_{k+2}}\Phi^{(k+1)}(x_1, \dots, x_{k+1}, X_{k+2}, \dots, X_n), \tag{21}$$

$$\partial_{x_{n-1}}\Phi^{(n-1)}(x_1, \dots, x_{n-1}, X_n) = x_n, \tag{22}$$

for $k = 1, \dots, n-2$.

Remark 4. As in Remark 3, choosing $\Phi^{(i)} = x_iX_{i+1}$ in (20)-(22) generates the identity map.

2.2. **First order volume preserving mappings.** In this subsection, we focus on the construction of first-order volume preserving integrators for divergence free differential equations using (19) and (20)–(22). As already mentioned in Section 1.1, these conditions need be associated to a specific representation of the given vector field (1) to give meaningful numerical maps. We will identify the representation of the vector field $\mathbf{a}(\mathbf{x})$ in (1) naturally associated to (20)-(22), as

$$\begin{aligned}
\dot{x}_1 =& \partial_{x_2}F^{(1)}(x_1, x_2, \dots, x_n), \\
\dot{x}_2 =& -\partial_{x_1}F^{(1)}(x_1, x_2, \dots, x_n) + \partial_{x_3}F^{(2)}(x_1, x_2, \dots, x_n), \\
&\vdots \\
\dot{x}_{n-1} =& -\partial_{x_{n-2}}F^{(n-2)}(x_1, x_2, \dots, x_n) + \partial_{x_n}F^{(n-1)}(x_1, x_2, \dots, x_n), \\
\dot{x}_n =& -\partial_{x_{n-1}}F^{(n-1)}(x_1, x_2, \dots, x_n).
\end{aligned} \tag{23}$$

The above representation of a divergence free vector field was proposed by Feng and his co-authors [6, 5, 16], and is just one of the many possible. A priori, it is not immediate to determine which representation is most natural for a given couple of differential forms $(\nu, \tilde{\nu})$ and for this reason, it is illustrative to describe a general procedure. For every divergence free field $\mathbf{a} = (a_1, a_2, \ldots, a_n)^T$, there corresponds an anti-symmetric tensor field $B = (b_{i,j})_{i,j=1,\ldots,n}, b_{i,j} = -b_{j,i}$, such that

$$a_i = \sum_{j=1}^{n} \frac{\partial b_{i,j}}{\partial x_j}, \ i = 1, \ldots, n.$$

Now, (1) becomes

$$\dot{x}_i = \sum_{j=1}^{n} \frac{\partial b_{i,j}}{\partial x_j}, \ b_{i,j} = -b_{j,i}, \ i = 1, \ldots, n. \tag{24}$$

The matrix B can be split into skew-symmetric sub-matrices,

$$\begin{aligned} B = & \begin{pmatrix} 0 & b_{1,2} & 0 & \ldots & 0 \\ -b_{1,2} & 0 & 0 & \ldots & 0 \\ 0 & 0 & 0 & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots & \\ 0 & 0 & 0 & \ldots & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & b_{1,3} & \ldots & 0 \\ 0 & 0 & 0 & \ldots & 0 \\ -b_{1,3} & 0 & 0 & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots & \\ 0 & 0 & 0 & \ldots & 0 \end{pmatrix} + \ldots \\ = & \ B^{1,2} + B^{1,3} + \cdots + B^{n-1,n}, \end{aligned} \tag{25}$$

which are not uniquely determined (there are $n(n-1)/2$ such matrices for a system of dimension n).[2] Feng and Shang [5] proposed Weyl's normalization [20], with

$$\begin{aligned} b_{1,2} &= \int_0^{x_2} a_1(x_1, s_2, x_3, \ldots, x_n) ds_2, \\ b_{k,k+1} &= \int_0^{x_{k+1}} (a_k + \frac{\partial b_{k-1,k}}{\partial x_{k-1}})(x_1, \ldots, x_k, s_{k+1}, x_{k+2}, \ldots, x_n) ds_{k+1}, \\ & \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad 2 \le k \le n-2, \\ b_{n-1,n} &= \int_0^{x_n} (a_{n-1} + \frac{\partial b_{n-2,n-1}}{\partial x_{n-2}})(x_1, \ldots, x_{n-1}, s_n) ds_n \\ & \qquad - \int_0^{x_{n-1}} a_n(x_1, \ldots, x_{n-2}, s_{n-1}, 0) ds_{n-1}, \end{aligned}$$

and all the other elements $b_{i,j} = 0$. Thus, the divergence free differential equation can be written as

$$\begin{aligned} \dot{x}_1 &= \frac{\partial b_{1,2}}{\partial x_2}, \\ \dot{x}_2 &= -\frac{\partial b_{1,2}}{\partial x_1} + \frac{\partial b_{2,3}}{\partial x_3}, \\ &\vdots \\ \dot{x}_{n-1} &= -\frac{\partial b_{n-2,n-1}}{\partial x_{n-2}} + \frac{\partial b_{n-1,n}}{\partial x_n}, \\ \dot{x}_n &= -\frac{\partial b_{n-1,n}}{\partial x_{n-1}}. \end{aligned}$$

Setting $F^{(1)} = b_{1,2}$, $F^{(2)} = b_{2,3}$, $\ldots$, $F^{(n-1)} = b_{n-1,n}$, we recover (23).

[2] McLachlan and Quispel [12] gave another way to construct tensor field in Appendix A, page 429-430.

Theorem 2.2. *Given (23), the $(n-2)$ generating form (19) generates a canonical transformation $\mathbf{f} : (x_1, \ldots, x_n) \mapsto (X_1, \ldots, X_n)$. Further, the choice*

$$\Phi^{(r)}(x_1, \ldots, x_r, X_{r+1}, \ldots, X_n) = x_r X_{r+1} + \Delta t F^{(r)}(x_1, \ldots, x_r, X_{r+1}, \ldots, X_n) \quad (26)$$

yields the first order volume preserving method for (23),

$$\begin{aligned}
X_1 &= x_1 + \Delta t \partial_{X_2} F^{(1)}(x_1, X_2, \ldots, X_n),\\
X_2 &= x_2 - \Delta t \partial_{x_1} F^{(1)}(x_1, X_2, \ldots, X_n) + \Delta t \partial_{X_3} F^{(2)}(x_1, x_2, X_3, \ldots, X_n),\\
&\vdots\\
X_{n-1} &= x_{n-1} - \Delta t \partial_{x_{n-2}} F^{(n-2)}(x_1, \ldots, x_{n-2}, X_{n-1}, X_n)\\
&\qquad + \Delta t \partial_{X_n} F^{(n-1)}(x_1, \ldots, x_{n-1}, X_n),\\
X_n &= x_n - \Delta t \partial_{x_{n-1}} F^{(n-1)}(x_1, \ldots, x_{n-1}, X_n),
\end{aligned}$$

where Δt is the time step of integration.

Proof. The choice of functions (26) obviously satisfies (20)–(22), which give directly the above mentioned numerical method. Details about how the functions $\Phi^{(r)}$ are derived from (20)–(22) can be found in Appendix B. □

In other words, it is the generating form that dictates the normalization of the divergence free vector field. Thus, a normalization of the type

$$\begin{aligned}
\dot{x}_1 &= \partial_{x_n} F^{(1)}(x_1, x_2, \ldots, x_n),\\
\dot{x}_2 &= \partial_{x_n} F^{(2)}(x_1, x_2, \ldots, x_n),\\
&\vdots\\
\dot{x}_{n-1} &= \partial_{x_n} F^{(n-1)}(x_1, x_2, \ldots, x_n),\\
\dot{x}_n &= -\sum_{i=1}^{n-1} \partial_{x_i} F^{(i)}(x_1, x_2, \ldots, x_n),
\end{aligned}$$

does not fit in (20)–(22).

Remark 5. The method of Theorem 2.2 is the n-variables equivalent of the (123, 231) *A*-*D* case in Table 2, corresponds to $\nu = (-1)^{n-1} x_n dx_1 \wedge \cdots \wedge dx_{n-1}$, $\tilde{\nu} = x_1 dx_2 \wedge \cdots \wedge dx_n$, and is associated to the Weyl normalization (23). The other cases in (11) can be obtained by cyclic permutations of the indices and are the $\nu \neq \tilde{\nu}$ cases that extend to n-dimensions in a straightforward manner.

As explained earlier, this gives a partial understanding of the connection between volume preserving generating forms and numerical methods. For instance, in the $n = 3$ case, for the table corresponding to $(123, 231)$, there are still three cases, *A*-*C*, *B*-*C*, *B*-*D* for which the connection between the vector field and generating forms is not yet well understood and currently under investigation [21].

The result of the above theorem is not new insofar numerical methods are concerned. The volume preserving method in Theorem 2.2 can be interpreted as a composition of $n-1$ steps of a symplectic Euler applied to a splitting of the vector field (23) in $(n-1)$ two-dimensional Hamiltonians due to Feng and Shang (see also [8], pp. 230–231). The splitting of a divergence free vector field in two-dimensional Hamiltonians, each approximated by a symplectic method, was one of the earliest techniques to obtain volume preserving integrators. See also [16] for a further discussion about this method and an extensive discussion on local structures.

3. **Extension of Poincaré's generating function.** We review Poincaré's generating function [19] for symplectic maps. Inspired by the form (29) of Poincaré's generating function and using linear transformations, we obtain more general generating 0-forms (functions) for the symplectic case. The generating 0-form has the symplectic Euler-A method, the symplectic Euler-B method and the Implicit Midpoint Rule method as special cases. Thereafter, we extend such generalization to the case of volume forms.

3.1. **Symplectic maps.** Consider the vicinity of the point $\mathbf{0}$ in a $2n$ dimensional manifold $\mathcal{M}$ with a canonical symplectic structure ω,

$$\omega = \sum_{i=1}^{n} dx_i \wedge dx_{n+i}.$$

Introducing the skew-symmetric $2n \times 2n$ matrix $[\omega_{ij}]$ defined as

$$\omega_{ij} = \begin{cases} 0 & i \neq j \pm n, \\ 1 & i = j - n, \\ -1 & i = j + n, \end{cases}$$

one can rewrite the symplectic structure as

$$\omega = \frac{1}{2} \sum_{i,j=1}^{2n} \omega_{ij} dx_i \wedge dx_j. \tag{27}$$

Recall from Section 1 that a canonical transformation $\mathbf{f} : \mathbf{x} \in \mathcal{V} \mapsto \mathbf{X} \in \mathcal{M}$, where $\mathcal{V}$ is an open neighborhood of $\mathbf{0}$ in $\mathcal{M}$, satisfies $\mathbf{f}^*\omega = \omega$. Now, rewrite the $\mathbf{f}^*\omega - \omega = 0$ as

$$L = \frac{1}{2} \sum_{i,j=1}^{2n} \omega_{ij} [dX_i \wedge dX_j - dx_i \wedge dx_j] = 0. \tag{28}$$

There exists a 1-form $\phi_{\mathbf{x}}(\mathbf{f})$ such that $d\phi_{\mathbf{x}}(\mathbf{f}) = L$, where

$$\phi_{\mathbf{x}}(\mathbf{f}) = \sum_{i,j=1}^{2n} \omega_{ij} (X_i - x_i) d[\frac{1}{2}(X_j + x_j)]. \tag{29}$$

Since $d\phi_{\mathbf{x}}(\mathbf{f}) = L = 0$, there is an uniquely determined function $S_{\mathbf{x}}(\mathbf{f}) : \mathcal{V} \longrightarrow \mathbf{R}$ such that $S_{\mathbf{x}}(\mathbf{f})(\mathbf{0}) = 0$ and $dS_{\mathbf{x}}(\mathbf{f}) = \phi_{\mathbf{x}}(\mathbf{f})$.

Definition 3.1. [19]. Given $\phi_{\mathbf{x}}(\mathbf{f})$ as in (29), the function $S_{\mathbf{x}}(\mathbf{f})$ such that $dS_{\mathbf{x}} = \phi_{\mathbf{x}}(\mathbf{f})$, is called Poincaré's generating function for $\mathbf{f}$, relative to the canonical coordinate system $\mathbf{x}$.

We illustrate the two dimensional case in detail, the generalization to the n-dimensional case is straightforward. To use the standard symplectic notation, we set $p = x_1, q = x_2, P = X_1$ and $Q = X_2$. Assume that the map $\mathbf{f} : (q, p) \mapsto (Q, P)$ is a canonical transformation, that is $dP \wedge dQ = dp \wedge dq$. Then, (29) becomes

$$\phi_{(p,q)}(\mathbf{f}) = (P - p)d[\frac{1}{2}(Q + q)] - (Q - q)d[\frac{1}{2}(P + p)].$$

Set

$$\begin{aligned}\tilde{P} =& P - p,\\ \tilde{Q} =& \frac{Q+q}{2},\\ \tilde{q} =& -Q + q,\\ \tilde{p} =& \frac{P+p}{2},\end{aligned} \tag{30}$$

then $\phi_{(p,q)}(\mathbf{f})$ becomes

$$\phi_{(p,q)}(\mathbf{f}) = \tilde{P}d\tilde{Q} + \tilde{q}d\tilde{p}.$$

This corresponds to the choice of primitives $\tilde{p}d\tilde{q}$ and $-\tilde{q}d\tilde{p}$ in Table 1, hence to generating functions of type II. in the ($\tilde{\ }$)-variables. Thus, there exists a function S (the same as the *Poincare's generating function* $S_{\mathbf{x}}$ of Definition 3.1 when considered a function in the regular variables) such that

$$\tilde{P}d\tilde{Q} + \tilde{q}d\tilde{p} = dS(\tilde{P}, \tilde{Q}, \tilde{p}, \tilde{q}). \tag{31}$$

From the left side of (31), we have $dS(\tilde{P}, \tilde{Q}, \tilde{p}, \tilde{q}) = \partial_{\tilde{P}}Sd\tilde{P} + \partial_{\tilde{Q}}Sd\tilde{Q} + \partial_{\tilde{p}}Sd\tilde{p} + \partial_{\tilde{q}}Sd\tilde{q}$. By comparing both sides of (31), we can see that the function S depends only on $\tilde{p}$ and $\tilde{Q}$, and

$$\begin{aligned}\tilde{P} =& \partial_{\tilde{Q}}S(\tilde{p}, \tilde{Q}),\\ \tilde{q} =& \partial_{\tilde{p}}S(\tilde{p}, \tilde{Q}).\end{aligned} \tag{32}$$

Easily, we obtain the relations

$$\begin{aligned}P - p =& \partial_2 S(\frac{P+p}{2}, \frac{Q+q}{2}),\\ Q - q =& -\partial_1 S(\frac{P+p}{2}, \frac{Q+q}{2}).\end{aligned} \tag{33}$$

Here ∂_1 is the partial derivative with respect to the first variable $\tilde{p}$, while ∂_2 is the partial derivative with respect to the second variable $\tilde{Q}$. The above equations (33) generate the identity map for $S = 0$. The relations (33) generate the well known implicit midpoint rule method (IMR), which is a symplectic method. See also [15, 8].

3.2. Generalization of Poincaré's generating function for the symplectic case.

We observe that the $\tilde{Q}$ and $\tilde{q}$ in (30) are linear combinations of Q and q, and $\tilde{P}$ and $\tilde{p}$ are linear combinations of P and p. We search for more general methods by considering the linear transformation,

$$\begin{aligned}\tilde{P} =& \alpha_1 P + \alpha_2 p,\\ \tilde{p} =& \gamma_1 P + \gamma_2 p,\\ \tilde{Q} =& \beta_1 Q + \beta_2 q,\\ \tilde{q} =& \delta_1 Q + \delta_2 q,\end{aligned} \tag{34}$$

where $\alpha_1, \alpha_2, \beta_1, \beta_2, \gamma_1, \gamma_2, \delta_1, \delta_2$ are some coefficients to be determined. We look for coefficients such that

$$d\tilde{P} \wedge d\tilde{Q} - d\tilde{p} \wedge d\tilde{q} = dP \wedge dQ - dp \wedge dq. \tag{35}$$

Thus,

$$d\tilde{P} \wedge d\tilde{Q} - d\tilde{p} \wedge d\tilde{q} = 0,$$

implies

$$dP \wedge dQ - dp \wedge dq = 0. \tag{36}$$

The transformation from the original variables to the ($\tilde{}$)-variables need not be canonical. Thus (35) is a simplifying condition, as it allows us to generate a symplectic map $(\tilde{p}, \tilde{q}) \mapsto (\tilde{P}, \tilde{Q})$ with any of the known techniques for the generating functions in Table 1. For consistency with the approach in the previous subsection (cfr. also Remark 3), we consider a map obeying (31) (symplectic generating functions type II.)

The condition for the Poincaré generating function to be consistent with the identity map was that $\tilde{P}, \tilde{q} \to 0$ when $(P, Q) \to (p, q)$. In our setting, this translates to

$$\alpha_1 = -\alpha_2 = \theta,$$
$$\delta_1 = -\delta_2 = \eta,$$

where θ and η are some constants. Hence, we have

$$\begin{aligned} d\tilde{P} \wedge d\tilde{Q} - d\tilde{p} \wedge d\tilde{q} &= (\theta\beta_1 - \gamma_1\eta)dP \wedge dQ + (-\theta\beta_1 - \eta\gamma_2)dp \wedge dQ \\ &+ (\theta\beta_2 + \eta\gamma_1)dP \wedge dq + (-\theta\beta_2 + \eta\gamma_2)dp \wedge dq \\ &= dP \wedge dQ - dp \wedge dq. \end{aligned}$$

Comparing both sides of the above equations, we deduce

$$\begin{pmatrix} \theta & 0 & -\eta & 0 \\ 0 & -\theta & 0 & \eta \\ 0 & \theta & \eta & 0 \\ \theta & 0 & 0 & \eta \end{pmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \gamma_1 \\ \gamma_2 \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \\ 0 \\ 0 \end{pmatrix}.$$

Both the matrix and the augmented matrix of the above linear system have rank 3, therefore there exists a one-parameter family of solutions to the above linear equation. Setting $\gamma_2 = -\epsilon$, we have

$$\begin{pmatrix} \tilde{P} \\ \tilde{Q} \\ \tilde{p} \\ \tilde{q} \end{pmatrix} = \begin{pmatrix} \theta & 0 & -\theta & 0 \\ 0 & \frac{\eta\epsilon}{\theta} & 0 & 1 - \frac{\eta\epsilon}{\theta} \\ \epsilon - \frac{1}{\eta} & 0 & -\epsilon & 0 \\ 0 & \eta & 0 & -\eta \end{pmatrix} \begin{pmatrix} P \\ Q \\ p \\ q \end{pmatrix}. \tag{37}$$

By changing $\tilde{p} \mapsto -\tilde{p}$, (32) becomes

$$\begin{aligned} \tilde{P} &= \partial_{\tilde{Q}} S(\tilde{p}, \tilde{Q}), \\ \tilde{q} &= -\partial_{\tilde{p}} S(\tilde{p}, \tilde{Q}). \end{aligned}$$

In conclusion, we obtain the following family of symplectic methods.

Theorem 3.2. *For any $\theta, \eta \neq 0$ and any ϵ, the scheme*

$$\begin{aligned} P &= p + \frac{1}{\theta}\partial_2 S((\frac{1}{\eta} - \epsilon)P + \epsilon p, \frac{\eta\epsilon}{\theta}Q + \frac{1 - \eta\epsilon}{\theta}q), \\ Q &= q - \frac{1}{\eta}\partial_1 S((\frac{1}{\eta} - \epsilon)P + \epsilon p, \frac{\eta\epsilon}{\theta}Q + \frac{1 - \eta\epsilon}{\theta}q). \end{aligned} \tag{38}$$

generates a canonical transformation.

In the context of numerical integration, the constants θ, η in (38) should be close to 1 to have consistent numerical methods.

There are some special cases which are very interesting to study.

Corollary 1 (Two-parameter-family of symplectic Euler methods)**.** *The symplectic schemes*

$$P = p + \frac{1}{\theta}\partial_2 S(\frac{1}{\eta}P, \frac{1}{\theta}q), \quad Q = q - \frac{1}{\eta}\partial_1 S(\frac{1}{\eta}P, \frac{1}{\theta}q) \tag{39}$$

$$P = p + \frac{1}{\theta}\partial_2 S(\frac{1}{\eta}p, \frac{1}{\theta}Q), \quad Q = q - \frac{1}{\eta}\partial_1 S(\frac{1}{\eta}p, \frac{1}{\theta}Q). \tag{40}$$

have the symplectic Euler B and A methods, respectively, as the special case.

Proof. In both cases, let $S = -\Delta t H$, where H is the Hamiltonian function of the system, and let $\theta = \eta = 1$. When setting $\epsilon = 0$ in (38), we recover the symplectic Euler B, while setting $\epsilon = \frac{1}{\eta}$, we obtain the symplectic Euler A. □

Corollary 2 (Symplectic theta method)**.** *For any choice of ϑ, the scheme*

$$\begin{aligned} P =& p + \partial_2 S(\vartheta P + (1-\vartheta)p, (1-\vartheta)Q + \vartheta q), \\ Q =& q - \partial_1 S(\vartheta P + (1-\vartheta)p, (1-\vartheta)Q + \vartheta q), \end{aligned} \tag{41}$$

is symplectic. Moreover, letting $S = -\Delta t H$, the choices $\vartheta = \frac{1}{2}, 1, 0$ yield the IMR, the symplectic Euler A and B respectively.

Proof. The proof follows immediately from (38): choosing $\theta = \eta = 1$ and ϵ to $1 - \vartheta$ □

In passing, we mention that a particular case of the above symplectic theta method (41) for separable Hamiltonian systems was derived in [10] using the framework of discrete Lagrangians.

3.3. **Extension to volume preserving mappings.** Following the procedure of last subsection, we use the technique of changing variables by linear transformations. Let $M = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \in GL(2n)$, where A, B, C, D some arbitrary $n \times n$ matrices. Consider change of variables $(x_1, x_2, \ldots, x_n) \mapsto (\tilde{x}_1, \tilde{x}_2, \ldots, \tilde{x}_n)$ and $(X_1, X_2, \ldots, X_n) \mapsto (\tilde{X}_1, \tilde{X}_2, \ldots \tilde{X}_n)$ given by

$$\begin{pmatrix} \tilde{\mathbf{X}} \\ \tilde{\mathbf{x}} \end{pmatrix} = M \begin{pmatrix} \mathbf{X} \\ \mathbf{x} \end{pmatrix} \tag{42}$$

where $\mathbf{X} = (X_1, X_2, \ldots, X_n)^T$, $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$, $\tilde{\mathbf{X}} = (\tilde{X}_1, \tilde{X}_2, \ldots \tilde{X}_n)^T$ and $\tilde{\mathbf{x}} = (\tilde{x}_1, \tilde{x}_2, \ldots, \tilde{x}_n)^T$. Such linear variable transformations have been used at great length by Feng and Shang, see [17]. In their derivation of the methods, they do not use differential forms, but the equivalent condition (5) directly. The generic case is very hard to tackle with, because of the large number of unknowns, hence simplifying conditions are needed. Shang [17] requires a Hadamard matrix condition. Our simplifying condition is the equivalent of (35), as explained in the lemma below.

Lemma 3.3 (Simplifying condition)**.** *Assume that the map $(\tilde{x}_1, \tilde{x}_2, \ldots, \tilde{x}_n) \mapsto (\tilde{X}_1, \tilde{X}_2, \ldots \tilde{X}_n)$ satisfies*

$$\wedge^n \tilde{\mathbf{X}} - \wedge^n \tilde{\mathbf{x}} = 0 \tag{43}$$

where $\wedge^n \mathbf{X} = dX_1 \wedge dX_2 \wedge \cdots \wedge dX_n$. If

$$\wedge^n \tilde{\mathbf{X}} - \wedge^n \tilde{\mathbf{x}} = \wedge^n \mathbf{X} - \wedge^n \mathbf{x}, \tag{44}$$

then

$$\wedge^n \mathbf{X} - \wedge^n \mathbf{x} = 0. \tag{45}$$

i.e. the map $\mathbf{f} : \mathbf{x} \mapsto \mathbf{X}$ is volume preserving.

Because of Remark 5, it is sufficient to analyze the n dimensional case with

$$\nu = (-1)^{n-1} x_n dx_1 \wedge \cdots \wedge dx_{n-1}, \qquad \tilde{\nu} = x_1 dx_2 \wedge \cdots \wedge dx_n, \tag{46}$$

associated to the Weyl normalization (23). We commence with the $n = 3$ case. The following negative result holds.

Theorem 3.4. *Let $n = 3$. Consider an implicitly defined transformation (42) with A, B, C, D diagonal matrices. There is no nonzero choice of coefficients in the matrices that is consistent with the identity map and satisfies the simplifying conditions (43).*

Proof. We write the implicitly defined transformation as

$$\begin{pmatrix} \tilde{X}_1 \\ \tilde{X}_2 \\ \tilde{X}_3 \\ \tilde{x}_1 \\ \tilde{x}_2 \\ \tilde{x}_3 \end{pmatrix} = \begin{pmatrix} \alpha_1 & 0 & 0 & \beta_1 & 0 & 0 \\ 0 & \alpha_2 & 0 & 0 & \beta_2 & 0 \\ 0 & 0 & \alpha_3 & 0 & 0 & \beta_3 \\ \gamma_1 & 0 & 0 & \delta_1 & 0 & 0 \\ 0 & \gamma_2 & 0 & 0 & \delta_2 & 0 \\ 0 & 0 & \gamma_3 & 0 & 0 & \delta_3 \end{pmatrix} \begin{pmatrix} X_1 \\ X_2 \\ X_3 \\ x_1 \\ x_2 \\ x_3 \end{pmatrix}, \tag{47}$$

and consider (46) in the ($\tilde{\ }$)-variables, for which solutions are known, see Theorem 2.2. Without loss of generality, we can assume (the same principle as for the symplectic case),

$$\begin{aligned} \alpha_1 = 1,\ \beta_1 = -1, \\ \gamma_3 = 1,\ \delta_3 = -1. \end{aligned} \tag{48}$$

The simplifying conditions (43) yield a set of 8 quadratic equations in 8 unknowns. It can be shown by direct computation that the nonzero solution are not compatible with (48). □

Lemma 3.5. *Let $n = 3$ and assume that the transformation matrix M in (42) has the block diagonal form*

$$M = \begin{pmatrix} \Delta_1 & \mathbf{0} \\ \mathbf{0} & \Delta_2 \end{pmatrix}.$$

*(**First class**). The following choices of Δ_i, $i = 1, 2$,*

$$\begin{pmatrix} \frac{1}{\theta_i} & & \\ & \theta_i & \\ & & 1 \end{pmatrix} \begin{pmatrix} 0 & \frac{1}{\theta_i} & 0 \\ 0 & 0 & \theta_i \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & \frac{1}{\theta_i} \\ \theta_i & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & \frac{1}{\theta_i} \\ 0 & -\theta_i & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & \frac{1}{\theta_i} & 0 \\ -\theta_i & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

($\theta_i \neq 0$), obey the simplifying condition (44), hence yield volume preserving methods.

Similarly, if M has the form

$$M = \begin{pmatrix} \mathbf{0} & \Delta_3 \\ \Delta_4 & \mathbf{0} \end{pmatrix},$$

*(**Second class**), the choices*

$$\begin{pmatrix} \frac{-1}{\theta_i} & & \\ & \theta_i & \\ & & 1 \end{pmatrix} \begin{pmatrix} 0 & \frac{1}{\theta_i} & 0 \\ 0 & 0 & -\theta_i \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & \frac{1}{\theta_i} \\ -\theta_i & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & \frac{1}{\theta_i} \\ 0 & \theta_i & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & \frac{1}{\theta_i} & 0 \\ \theta_i & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

($\theta_i \neq 0$), also obey the simplifying conditions (44) and yield canonical (volume preserving) transformations.

Proof. For the case of **First class**, the form of Δ_1 implies

$$\begin{array}{lllll} \tilde{X}_1 = \frac{1}{\theta_1}X_1, & \tilde{X}_1 = \frac{1}{\theta_1}X_2, & \tilde{X}_1 = \frac{1}{\theta_1}X_3, & \tilde{X}_1 = \frac{1}{\theta_1}X_3, & \tilde{X}_1 = \frac{1}{\theta_1}X_2, \\ \tilde{X}_2 = \theta_1 X_2, & \tilde{X}_2 = \theta_1 X_3, & \tilde{X}_2 = \theta_1 X_1, & \tilde{X}_2 = -\theta_1 X_2, & \tilde{X}_2 = -\theta_1 X_1, \\ \tilde{X}_3 = X_3, & \tilde{X}_3 = X_1, & \tilde{X}_3 = X_2, & \tilde{X}_3 = X_1, & \tilde{X}_3 = X_3, \end{array}$$

and it is easily verified that $d\tilde{X}_1 \wedge d\tilde{X}_2 \wedge d\tilde{X}_3 = dX_1 \wedge dX_2 \wedge dX_3$. Similarly, the forms of Δ_2 imply that $d\tilde{x}_1 \wedge d\tilde{x}_2 \wedge d\tilde{x}_3 = dx_1 \wedge dx_2 \wedge dx_3$. Obviously, (44) is satisfied by matrices of the **First class**.

With the same procedure, we can easily see that the forms of Δ_3 imply $d\tilde{X}_1 \wedge d\tilde{X}_2 \wedge d\tilde{X}_3 = -dx_1 \wedge dx_2 \wedge dx_3$ and the forms of Δ_4 imply $d\tilde{x}_1 \wedge d\tilde{x}_2 \wedge d\tilde{x}_3 = dX_1 \wedge dX_2 \wedge dX_3$, and (44) is also satisfied by matrices of **Second class**. □

The following theorem holds.

Theorem 3.6. *Given the divergence free differential equation*

$$\begin{aligned} \dot{x}_1 &= \partial_{x_2} F^{(1)}(x_1, x_2, x_3), \\ \dot{x}_2 &= -\partial_{x_1} F^{(1)}(x_1, x_2, x_3) + \partial_{x_3} F^{(2)}(x_1, x_2, x_3), \\ \dot{x}_3 &= -\partial_{x_2} F^{(2)}(x_1, x_2, x_3), \end{aligned}$$

the method

$$\begin{aligned} X_1 &= x_1 + \frac{\Delta t}{\theta_2}\partial_{x_2} F^{(1)}(\frac{1}{\theta_1}X_1, \theta_2 x_2, \frac{1}{\theta_2}x_3), \\ X_2 &= x_2 - \frac{\Delta t}{\theta_2}\partial_{X_1} F^{(1)}(\frac{1}{\theta_1}X_1, \theta_2 x_2, \frac{1}{\theta_2}x_3) + \frac{\Delta t}{\theta_1}\partial_{x_3} F^{(2)}(\frac{1}{\theta_1}X_1, \theta_1 X_2, \frac{1}{\theta_2}x_3), \\ X_3 &= x_3 - \frac{\Delta t}{\theta_1}\partial_{X_2} F^{(2)}(\frac{1}{\theta_1}X_1, \theta_1 X_2, \frac{1}{\theta_2}x_3), \end{aligned}$$

is volume preserving. Moreover, if $\theta_1, \theta_2 = 1 + O(\Delta t)$, the method has order at least one.

Proof. In order to obtain the volume preserving numerical schemes, we choose the matrix M as the First class as

$$\Delta_1 = \begin{pmatrix} \frac{1}{\theta_1} & & \\ & \theta_1 & \\ & & 1 \end{pmatrix}, \quad \Delta_2 = \begin{pmatrix} 1 & & \\ & \theta_2 & \\ & & \frac{1}{\theta_2} \end{pmatrix}.$$

Then, (42) implies,

$$\begin{aligned} \tilde{X}_1 &= \frac{1}{\theta_1}X_1, & \tilde{x}_1 &= x_1, \\ \tilde{X}_2 &= \theta_1 X_2, & \tilde{x}_2 &= \theta_2 x_2, \\ \tilde{X}_3 &= X_3, & \tilde{x}_3 &= \frac{1}{\theta_2}x_3. \end{aligned} \tag{49}$$

Because of Remark 5, we have the generating one-form

$$\lambda = B(\tilde{X}_1, \tilde{x}_2, \tilde{x}_3)d\tilde{x}_3 + C(\tilde{X}_1, \tilde{X}_2, \tilde{x}_3)d\tilde{X}_1. \tag{50}$$

(case (231,123) B-C, see Table 2, or [11]). Theorem 2.2 holds in the (˜)-variables. Thus the first part of the statement follows immediately by substituting (49) in place of the (˜)-variables.

For the order statement, note that for $\theta_1 = \theta_2 = 1$ we recover precisely the adjoint method of Theorem 2.2 for $\mathbf{R}^3$ (case (123,231) A-D), which is a composition of symplectic Euler steps and has order one. Clearly, as long as $\theta_i = 1 + O(\Delta t)$, $i = 1, 2$, the order of the method (49) is at least one. □

For the $\mathbf{R}^n$ case, the matrix M has similar structure as the three dimensional case and similar techniques can be used to obtain the generating forms and the numerical schemes. From Lemma 3.5 and its proof, we see that there can be up to $2(n-2)$ coefficients for each of the two classes. Different ways of choosing those coefficients and matrix forms gives us different M's. For instance, if we choose M in the first class, with

$$\Delta_1 = \begin{pmatrix} \frac{1}{\theta_1} & & & & & \\ & \theta_1 & & & & \\ & & 1 & & & \\ & & & 1 & & \\ & & & & \cdots & \\ & & & & & 1 \end{pmatrix}_{n\times n}, \quad \Delta_2 = \begin{pmatrix} 1 & & & & & \\ & \theta_2 & & & & \\ & & \frac{1}{\theta_2} & & & \\ & & & 1 & & \\ & & & & \cdots & \\ & & & & & 1 \end{pmatrix}_{n\times n}$$

then we can solve the divergence free differential equations (23) by the first order volume preserving scheme

$$\begin{aligned}
X_1 &= x_1 + \frac{\Delta t}{\theta_2}\partial_{x_2}F^{(1)}(\frac{X_1}{\theta_1}, \theta_2 x_2, \frac{x_3}{\theta_2}, x_4, \ldots, x_n),\\
X_2 &= x_2 - \frac{\Delta t}{\theta_2}\partial_{X_1}F^{(1)}(\frac{X_1}{\theta_1}, \theta_2 x_2, \frac{x_3}{\theta_2}, x_4, \ldots, x_n)\\
&\quad + \frac{\Delta t}{\theta_1}\partial_{x_3}F^{(2)}(\frac{X_1}{\theta_1}, \theta_1 X_2, \frac{x_3}{\theta_2}, x_4, \ldots, x_n),\\
X_3 &= x_3 - \frac{\Delta t}{\theta_1}\partial_{X_2}F^{(2)}(\frac{X_1}{\theta_1}, \theta_1 X_2, \frac{x_3}{\theta_2}, x_4, \ldots, x_n)\\
&\quad + \Delta t\partial_{x_4}F^{(3)}(\frac{X_1}{\theta_1}, \theta_1 X_2, X_3, x_4, \ldots, x_n),\\
X_4 &= x_4 - \Delta t\partial_{X_3}F^{(3)}(\frac{X_1}{\theta_1}, \theta_1 X_2, X_3, x_4, \ldots, x_n)\\
&\quad + \Delta t\partial_{x_5}F^{(4)}(\frac{X_1}{\theta_1}, \theta_1 X_2, X_3, X_4, \ldots, x_n),\\
&\vdots\\
X_{n-1} &= x_{n-1} - \Delta t\partial_{X_{n-2}}F^{(n-2)}(\frac{X_1}{\theta_1}, \theta_1 X_2, X_3 \ldots, X_{n-2}, x_{n-1}, x_n)\\
&\quad + \Delta t\partial_{x_n}F^{(n-1)}(\frac{X_1}{\theta_1}, \theta_1 X_2, X_3, \ldots, X_{n-1}, x_n),\\
X_n &= x_n - \Delta t\partial_{X_{n-1}}F^{(n-1)}(\frac{X_1}{\theta_1}, \theta_1 X_2, X_3, \ldots, X_{n-1}, x_n),
\end{aligned}$$

where Δt is time step and $\theta_1, \theta_2 = 1 + O(\Delta t)$. In general, we can choose any two $n \times n$ matrices

$$\Delta_1 = \begin{pmatrix} \theta_1 & & & & \\ & \theta_2 & & & \\ & & \cdots & & \\ & & & \theta_{n-1} & \\ & & & & 1 \end{pmatrix}, \quad \Delta_2 = \begin{pmatrix} 1 & & & & \\ & \eta_1 & & & \\ & & \eta_2 & & \\ & & & \cdots & \\ & & & & \eta_{n-1} \end{pmatrix}$$

subject to $\prod_{i=1}^{n-1}\theta_i = 1$ and $\prod_{i=1}^{n-1}\eta_i = 1$. For the divergence-free differential equation (23), we have a first order volume preserving scheme

$$\begin{aligned}
X_1 &= x_1 + \frac{1}{\eta_1}\Delta t\partial_{x_2}F^{(1)}(\theta_1 X_1, \eta_1 x_2, \ldots, \eta_{n-2}x_{n-1}, \eta_{n-1}x_n),\\
X_2 &= x_2 - \frac{1}{\eta_1}\Delta t\partial_{X_1}F^{(1)}(\theta_1 X_1, \eta_1 x_2, \ldots, \eta_{n-2}x_{n-1}, \eta_{n-1}x_n)\\
&\quad + \frac{\theta_1}{\eta_1\eta_2}\Delta t\partial_{x_3}F^{(2)}(\theta_1 X_1, \theta_2 X_2, \eta_2 x_3 \ldots, \eta_{n-2}x_{n-1}, \eta_{n-1}x_n),\\
&\vdots\\
X_{n-1} &= x_{n-1} - \frac{\eta_{n-1}\Delta t}{\theta_{n-2}\theta_{n-1}}\partial_{X_{n-2}}F^{(n-2)}(\theta_1 X_1, \ldots, \theta_{n-2}X_{n-2}, \eta_{n-2}x_{n-1}, \eta_{n-1}x_n)\\
&\quad + \frac{1}{\theta_{n-1}}\Delta t\partial_{x_n}F^{(n-1)}(\theta_1 X_1, \theta_2 X_2, \ldots, \theta_{n-1}X_{n-1}, \eta_{n-1}x_n),\\
X_n &= x_n - \frac{1}{\theta_{n-1}}\Delta t\partial_{X_{n-1}}F^{(n-1)}(\theta_1 X_1, \theta_2 X_2, \ldots, \theta_{n-1}X_{n-1}, \eta_{n-1}x_n).
\end{aligned}$$

As above, we require $\theta_i = 1 + O(\Delta t)$ and $\eta_i = 1 + O(\Delta t)$.

4. **Conclusion.** In this paper, we have presented a study of the generating function approach for symplectic and volume preserving mappings. Starting from [11], we have derived some classes of first order volume preserving methods through the differential forms assuming that the transformations are consistent with the identity map, recovering an approach already proposed by K. Feng using a decomposition in 2D Hamiltonians and symplectic methods.

We have then considered a generalization of Poincaré generating functions which generate IMR in the symplectic case. It is well known that the theta-method (weighted method)

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \Delta t\mathbf{f}((1-\vartheta)\mathbf{y}_n + \vartheta\mathbf{y}_{n+1}),$$

is symplectic if and only if $\vartheta = \frac{1}{2}$, as it coincides with the IMR [7]. In this paper, by extending Weinstein's definition [19] of Poincaré's generating function, we have obtained a symplectic generalization,

$$\begin{aligned}
\mathbf{p}_{n+1} &= \mathbf{p}_n + \Delta t\mathbf{f}_1(\vartheta\mathbf{p}_{n+1} + (1-\vartheta)\mathbf{p}_n, (1-\vartheta)\mathbf{q}_{n+1} + \vartheta\mathbf{q}_n)\\
\mathbf{q}_{n+1} &= \mathbf{q}_n + \Delta t\mathbf{f}_2(\vartheta\mathbf{p}_{n+1} + (1-\vartheta)\mathbf{p}_n, (1-\vartheta)\mathbf{q}_{n+1} + \vartheta\mathbf{q}_n)
\end{aligned}$$

where $\mathbf{y} = (\mathbf{p}, \mathbf{q})^T$ and $\mathbf{f} = (\mathbf{f}_1, \mathbf{f}_2)^T$. The symplectic theta method above is a (symplectic) partitioned Runge–Kutta method, and has the IMR, the symplectic Euler-A and B methods as special cases. We have adapted the approach to the volume preserving case, and, under some simplifying assumptions, we have found some new linear transformations which generate volume preserving methods. The general case is hard to investigate, because of the number of free parameters involved, and is far from being understood. In the future, we plan to investigate the other choices of differential forms and their connections with other classes of methods (like generating functions of type I. and discrete Lagrangians in the context of symplectic methods).

The methods presented in this paper are first order methods. There are several ways to obtain higher order methods. Besides the standard construction of composition by the adjoint method, it is possible to construct higher order methods using for instance the method of modified vector fields together with the conditions

(20)-(22), or the Hamilton–Jacobi differential equation. It is not obvious what are the Hamilton–Jacobi equations for these volume preserving forms. Although Shang [17] derived the Hamilton–Jacobi equation for his special class of volume preserving methods, it is not clear how these are related with the approach of differential forms presented here. We plan to investigate this issue in the future.

Acknowledgments. H.X. would like to thank J. Meiss, who introduced her to [11]. Both authors thank the IFS of Massey University for the hospitality received during their visits in Palmerston North in 2011, in particular Robert McLachlan for useful discussion and comments.

Appendix A. **Elements of differential calculus.** For convenience, we recall the definitions of differential form, wedge product and exterior derivative, and describe some of their most important properties.

Definition A.1 (Differential form)**.** Given a smooth manifold $\mathcal{M}$, a differential form ω of order k on $\mathcal{M}$ is a field of alternating k-linear maps. Denote $T_x\mathcal{M}$ the tangent space to $\mathcal{M}$ at x, then define

$$\omega_x : T_x\mathcal{M} \times \cdots \times T_x\mathcal{M} \mapsto \mathbf{R}$$

such that for all permutations σ of $\{1, \ldots, k\}$

$$\forall (u_1, \ldots, u_k) \in (T_x\mathcal{M})^k,\ \omega_x(u_{\sigma(1)}, \ldots, u_{\sigma(k)}) = \operatorname{sgn}(\sigma)\omega_x(u_1, \ldots, u_k)$$

where $\operatorname{sgn}(\sigma)$ denotes the sign of σ and ω_x is linear with respect to each augment u_i, $i = 1, \ldots, k$.

Definition A.2 (Wedge (or exterior) product)**.** The wedge product of a k-form ω and a l-form η on $\mathcal{M}$ is a $(k+l)$-form such that for all $x \in \mathcal{M}$ and for all $(u_1, \ldots, u_{k+l}) \in (T_x\mathcal{M})^{k+l}$,

$$(\omega \wedge \eta)_x(u_1, \ldots, u_{k+l}) = \sum_{\sigma \in S_{k,l}} \operatorname{sgn}(\sigma)\, \omega_x(u_{\sigma(1)}, \ldots, u_{\sigma(k)}) \cdot \eta_x(u_{\sigma(k+1)}, \ldots, u_{\sigma(k+l)}),$$

where the $S_{k,l}$ is the subset of permutations σ of $\{1, \ldots, k+l\}$, such that $\sigma(1) < \cdots < \sigma(k)$ and $\sigma(k+1) < \cdots < \sigma(k+l)$.

In particular, $\omega \wedge \eta = (-1)^{kl}\eta \wedge \omega$.

Definition A.3 (Pullback)**.** If f denotes a C^1 map from a smooth manifold $\mathcal{M}$ onto a smooth manifold $\mathcal{N}$, and ω a differential form of order k on $\mathcal{N}$, then the pullback of ω by f at x is defined as

$$\forall (u_1, \ldots, u_k) \in (T_x\mathcal{M})^k, (f^*\omega)_x(u_1, \ldots, u_k) = \omega_{f(x)}(df_x(u_1), \ldots, df_x(u_k)),$$

where df_x is the usual differential of f at x.

Definition A.4 (Exterior derivative)**.** The exterior derivative d is unique mapping of a k-form ω to $k+1$-form $d\omega$ on $\mathcal{M}$ such that:

1. If ω is a 0-form (i.e. $\omega = f$, where f is a function), then the one-form df is the differential of f.
2. d is linear, that is, $d(c_1\omega + c_2\eta) = c_1 d\omega + c_2 d\eta$.
3. If ω is k-form and η is l-form, $d(\omega \wedge \eta) = d\omega \wedge \eta + (-1)^k \omega \wedge d\eta$.

If ω is given in canonical coordinates as $\omega = \sum_{i_1<\cdots<i_k} \omega_{i_1,\ldots,i_k} dx_{i_1} \wedge \cdots \wedge dx_{i_k}$, then

$$d\omega = \sum_j \sum_{i_1<\cdots<i_k} \frac{\partial \omega_{i_1,\ldots,i_k}}{\partial x_j} dx_j \wedge dx_{i_1} \wedge \cdots \wedge dx_{i_k}.$$

The exterior derivative is natural with respect to the pullback, $d(f^*\omega) = f^* d\omega$. Moreover, for any k-form ω, it is true that

$$d^2\omega = d(d\omega) = 0.$$

Definition A.5 (Exact form and closed form)**.** A differential k-form ω is exact if there exists a $(k-1)$-form ν such that $\omega = d\nu$. Any such ν is also called a primitive (or potential form) of ω. A differential form ω is closed if $d\omega = 0$.

Thus, closed forms are the kernel of d, while exact forms are the image of d. Since $d^2 = 0$, any exact form is also closed (Poincaré lemma). Further, if $\mathcal{M}$ is simply connected, any closed form is also exact. In particular, if $\mathcal{M} = \mathbf{R}^n$, any closed form is exact.

The fundamental theorem of calculus generalizes to differential forms as Stoke's theorem:

$$\int_{\mathcal{S}} d\omega = \int_{\partial\mathcal{S}} \omega,$$

where $\partial\mathcal{S}$ is the oriented boundary of the oriented domain $\mathcal{S} \subseteq \mathcal{M}$.

Appendix B. Proof of Theorem 2.2.

Proof. Assume that the new variables $X_1, X_2, \ldots, X_n$ are close enough to the old ones $x_1, x_2, \ldots, x_n$ (we consider transformations which can generate the identity map, see Remark 1), that is,

$$\frac{\partial X_1}{\partial x_1}, \frac{\partial X_2}{\partial x_2}, \ldots, \frac{\partial X_n}{\partial x_n} = 1 + O(\Delta t), \tag{51}$$

for sufficiently small Δt. Similarly, assume for the inverse map, $\frac{\partial x_1}{\partial X_1}, \frac{\partial x_2}{\partial X_2}, \ldots, \frac{\partial x_n}{\partial X_n} = 1 + O(\Delta t)$.

Now, the first equation of (20) becomes

$$\partial_{x_1 X_2} \Phi^{(1)} = 1 + O(\Delta t).$$

We integrate both sides with respect to x_1 and X_2. Then, there exists an order $O(\Delta t)$ function $\psi^{(1)}$ such that

$$\Phi^{(1)} = x_1 X_2 + \psi^{(1)}(x_1, X_2, \ldots, X_n).$$

From the second equation of (20)-(22), we have

$$X_2 + \partial_{x_1} \psi^{(1)}(x_1, X_2, \ldots, X_n) = \partial_{X_3} \Phi^{(2)}(x_1, x_2, X_3, \ldots, X_n).$$

Integrating both sides with respect to X_3, and by noticing that $\Phi^{(2)}$ depends on the variables $x_1, x_2, X_3, \ldots, X_n$, we obtain

$$\begin{aligned} \Phi^{(2)} &= x_2 X_3 + \int (\partial_{x_1} \psi^{(1)}(x_1, x_2, X_3, \ldots, X_n) + O(\Delta t)) dX_3, \\ &= x_2 X_3 + \psi^{(2)}(x_1, x_2, X_3, \ldots, X_n), \end{aligned}$$

where

$$\psi^{(2)}(x_1, x_2, X_3, \ldots, X_n) = \int (\partial_{x_1} \psi^{(1)}(x_1, x_2, X_3, \ldots, X_n) + O(\Delta t)) dX_3.$$

Similarly, we can assume the functions $\psi^{(3)}, \dots, \psi^{(n-1)}$ such that

$$\begin{aligned} \Phi^{(3)} &= x_3 X_4 + \psi^{(3)}(x_1, x_2, x_3, X_4, \dots, X_n), \\ &\dots \\ \Phi^{(n-2)} &= x_{n-2} X_{n-1} + \psi^{(n-2)}(x_1, \dots, x_{n-2}, X_{n-1}, X_n), \\ \Phi^{(n-1)} &= x_{n-1} X_n + \psi^{(n-1)}(x_1, \dots, x_{n-1}, X_n). \end{aligned}$$

Substituting the above equations into (20)-(22), we obtain the new variables after time Δt

$$\begin{aligned} X_1 &= x_1 + \partial_{X_2} \psi^{(1)}(x_1, X_2, \dots, X_n), \\ X_2 &= x_2 - \partial_{x_1} \psi^{(1)}(x_1, X_2, \dots, X_n) + \partial_{X_3} \psi^{(2)}(x_1, x_2, X_3, \dots, X_n), \\ &\dots \\ X_{n-1} &= x_{n-1} - \partial_{x_{n-2}} \psi^{(n-2)}(x_1, \dots, x_{n-2}, X_{n-1}, X_n) \\ &+ \partial_{X_n} \psi^{(n-1)}(x_1, \dots, x_{n-1}, X_n), \\ X_n &= x_n - \partial_{x_{n-1}} \psi^{(n-1)}(x_1, \dots, x_{n-1}, X_n). \end{aligned}$$

By comparing the above equations with (23), we immediately see that by the choice $\psi^{(i)} = \Delta t F^{(i)},\ i = 1, \dots, n-1$, we obtain a volume preserving numerical scheme of (23) of order one. □

REFERENCES

[1] V. I. Arnold, "Mathematical Methods of Classical Mechanics," Springer, GMT 60, second edition, 1989.

[2] M. M. Carroll, *A representation theorem for volume preserving transformations*, J. International Journal of Non-Linear Mechanics, **39** (2004), 219–224.

[3] P. Chartier and A. Murua, *Preserving first integrals and volume forms of additively split systems*, IMA Journal of Numerical Analysis, **27** (2007), 381-C405.

[4] K. Feng, *Difference schemes for Hamiltonian formalism and symplectic geometry*, J. Comput. Math, **4** (1986), 279–289.

[5] K. Feng and Z.-J Shang, *Volume-preserving algorithms for source-free dynamical systems*, Numerische Mathematik, **71** (1995), 451–463.

[6] K. Feng and D.-L Wang, *Dynamical systems and geometric construction of algorithms*, Contemporary Mathematics, AMS, Providence, **163** (1994), 1–32.

[7] K. Feng, H. M. Wu, M.-Z. Qin and D.-L. Wang, *Construction of canonical difference schemes for Hamiltonian formalism via generating functions*, J. Comp. Math., **7** (1989), 71–96.

[8] E. Hairer, C. Lubich and G. Wanner, "Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations," Springer, Second edition, 2006.

[9] A. Iserles, G. R. W. Quispel and P. S. P. Tse, *B-series methods cannot be volume-reserving*, BIT Numerical Mathematics, **47** (2007), 351–378.

[10] J. E. Marsden and M. West, *Discrete mechanics and variational integrators*, Acta Numerica, **10** (2001), 357–514.

[11] H. E. Lomeli and J. D. Meiss, *Generating forms for exact volume preserving maps*, Discrete and Continuous Dynamical Systems serie S, **2** (2009), 361–377.

[12] R. I. McLachlan and G. R. W. Quispel, *Splitting methods*, Acta Numerica, **11** (2002), 341–434.

[13] J. Moser, "Notes on Dynamical System," Courant Lecture Notes in Mathematics, AMS, New York, 2005.

[14] J. Moser and A. P. Veselov, *Discrete version of some classical integrable systems and factorization of matrix polynomials*, Commun. Math. Phys., **139** (1991), 217–243.

[15] J. M. Sanz-Serna and M. P. Calvo, "Numerical Hamiltonian Problems," Chapman & Hall, 1994.

[16] Z.-J Shang, *Volume-preserving maps, source-free and their local structures*, J. Phys. A: Math. Gen., **39** (2006), 5601–5615.

[17] Z.-J Shang, "Generating Functions for Volume Preserving Mapping with Applications I: Basic Theory," China/Korea Joint Seminar: Dynamical Systems and Their Application, Available from: `http://www.mathnet.or.kr/mathnet/kms_tex/60105.pdf`.

[18] Z.-J Shang, *Construction of volume preserving difference schemes for source-free systems via generating function*, Journal of Computational Mathematics, **12** (1994), 265–272.

[19] A. Weinstein, *The invariance of Poincaré generating function for canonical transformations*, Inventiones math., **16** (1972), 202–213.

[20] H. Weyl, *The method of orthogonal projection in potential theory*, Duke Math. J., **7** (1940), 411–444.

[21] H. Xue, O. Verdier and A. Zanna, *Discrete Legendre transformation and volume preserving generating forms*, In Preparation, (2013).

[22] H. Xue and A. Zanna, *Explicit volume preserving splitting methods for polynomial divergence-free vector fields*, BIT Numerical Mathematics, **53** (2013), 265–281.

Received November 2012; revised February 2013.

E-mail address: `Huiyan.Xue@math.uib.no`
E-mail address: `Antonella.Zanna@math.uib.no`