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Generating functions for dynamical systems with symmetries, integrals, and differential invariants

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Abstract

We give a survey and some new examples of generating functions for systems with symplectic structure, systems with a first integral, systems that preserve volume, and systems with symmetries and/or time-reversing symmetries. Both ODEs and maps are treated, and we discuss how generating functions may be used in the structure-preserving numerical integration of ODEs with the above properties.

Keywords: Symplectic integrators; Volume-preserving; Generating functions

1. Introduction

Hamiltonian splitting is a widely applicable technique for numerically integrating Hamiltonian systems [11,23]. It yields methods that are symplectic, explicit, preserve simple integrals (such as bilinear and Casimir integrals), have good energy behaviour, and can be time-reversible with (spatial) reversing symmetries. The essential ingredient is to split the Hamiltonian rather than the vector field, thus automatically staying in the correct class of systems. Recently the basic idea underlying this method has been extended to classes of differential equations with more diverse structural properties, such as preservation of symmetries, integrals, eigenvalues, or phase space volume. In this paper we discuss how splitting, and numerical integration in general, depend on finding a *generating function form* (g.f.f.) for the class of systems at hand. The ideal case is to have similar generating functions available both for the differential equations and for the maps corresponding to their flows; but this is not always possible.

Here we survey generating functions for the above types of ODEs and maps, and discuss applications to structure-preserving integration methods. We also give some new examples: an energy and volume preserving method for

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Hamiltonian systems; a volume preserving method for flows on arbitrary manifolds, such as the three-torus; and a conserving method for many differential equations preserving volume and an integral. However, there are topological obstructions to applying the method to all such systems.

A generating function form for the space $\mathcal{S}$ of dynamical systems with a certain structure is a space $\mathcal{P}$, which we call the parameter space, and a function

$$g : \mathcal{P} \to \mathcal{S}, \ P \mapsto S. \tag{1}$$

In practice we want to compute g and manipulate objects in $\mathcal{P}$, for example by decomposing $P = \sum_i P_i$, so we usually take $\mathcal{P}$ to be a linear space such as the smooth functions $C^r(\mathbb{R}^m, \mathbb{R}^n)$. In some nice cases it is possible for g to be onto (every $s \in \mathcal{S}$ is generated by some parameter P) and/or 1–1 (no two distinct P's generate the same S). Unfortunately, these properties cannot be achieved in all cases of interest.

Two classical examples motivate this definition. Let $\mathcal{S}$ be the Hamiltonian vector fields, those whose flow preserves the canonical Hamiltonian structure

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}.$$

Let $\mathcal{P} = \{H \in C^2(\mathbb{R}^{2n}, \mathbb{R}): H(0) = 0\}$, where we have specified the arbitrary constant appearing in the Hamiltonian function H. Then a standard calculation shows that

$$g : H \mapsto J\nabla H \tag{2}$$

is a 1–1, onto generating function form in this sense: $g(H)$ is Hamiltonian for all H, and every Hamiltonian vector field is generated by a unique such H.

Secondly, there are many generating function forms for symplectic maps, the discrete-time analogue of Hamiltonian vector fields. [2,3] The classical type I, ..., IV forms and the Poincaré form

$$g : \mathcal{P} \to \mathrm{Symp}(\mathbb{R}^{2n}), \quad g(H) = \{x \mapsto x' : x' = x + J\nabla H((x + x')/2)\} \tag{3}$$

are members of a large class described by Ge [4]. In this class the space of generating function forms is itself parametrized by the symplectic maps on $\mathbb{R}^{4n}$. These g.f.f.'s are all locally 1–1 and onto, if the domain and range are restricted to suitable open neighbourhoods. (In applications to integrators one usually chooses a generating function form where the range includes the identity map. Also, in this application one includes a time step, which we here absorb in H throughout.) In this example, the parameter space $\mathcal{P}$ is the same for differential equations and for maps, and even g is fairly similar in the two cases.

Another large class of generating function forms for symplectic maps was only discovered with the advent of symplectic integration [23], and were previously unknown in classical mechanics. These are the symplectic Runge–Kutta methods,

$$x \mapsto x' = x + \sum_j b_j f(X_j), \tag{4}$$

[2] In addition, the form of Hamiltonian ODEs is invariant under symplectic maps. This is why such maps and their generating functions are also useful in manipulating and solving the ODEs. This second application of generating functions does not extend to other classes of systems.

[3] If KAM theory is to apply, we should further require that the maps be *exact symplectic* [24]. This is the case, for example, for flows of global Hamiltonian vector fields on exact symplectic manifolds.

where

$$X_i = x + \sum_j a_{ij} f(X_j), \quad i = 1, \ldots, s, \tag{5}$$

$$f = J\nabla H, \tag{6}$$

$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0 \tag{7}$$

for all i, j, and H is the generating function. (Does the Hamilton–Jacobi equation separate in any interesting cases for these forms?) One can even combine the ideas of this class and the previous one, getting a third class.

Unfortunately the situation for other classes of differential equations is not at all as clean. We shall see that we will be struggling to find generating function forms just for the differential equations themselves, let alone for their analogous maps. When there is a form g for the ODEs, one can regard exp, the time-1 flow of the differential equation,

$$\exp : P \mapsto \exp(g(P)) \tag{8}$$

as a generating function form. However, it does not usually map onto a whole neighbourhood of the identity, and nor is it computable in general.

It is useful to keep the diagram

$$\begin{array}{ccc} \dot{x} = f(x) & \longleftrightarrow & f = g(P) \\ \Big\downarrow \text{discretize} & & \Big\downarrow \text{discretize} \\ x \mapsto x' = \phi(x) & \longleftrightarrow & \phi = \tilde{g}(P) \end{array} \tag{9}$$

in mind, where the spaces on the right are linear and easy to work in. Of course, there is no general algorithm for discretizing generating function forms; so knowing the form for ODEs can only act as a guide to finding the form for maps.

Similar ideas are reviewed in [6,8], which include different applications, especially to systems on Lie groups and on similarity classes of matrices. Again the idea is to put coordinates on the 'difficult' space, in these cases a finite dimensional manifold rather than an infinite dimensional group of diffeomorphisms. In [6] it is also pointed out that the parameter space need not be linear, just some space in which it is easier to compute: a sphere for example.

A disadvantage of placing special coordinates on the space of interest is that if a system has more than one special property, the desired coordinates may conflict. Then one needs to find a generating function form for the intersection of the relevant spaces. This is attempted in Section 7, where special forms are given for systems preserving phase space volume *and* an integral.

Where possible we work on an arbitrary manifold M, using the language of differential geometry (see [14] for the notation). At a point $x \in M$ with tangent space $E = T_x M$, a k-form is a linear function $\alpha : E^k \to \mathbb{R}$ which is antisymmetric in all arguments. A k-vector is an antisymmetric linear function $K : E^{*k} \to \mathbb{R}$, i.e., it maps k 1-forms to the reals. Unfortunately, some of our constructions of maps can only be done in coordinates. Furthermore, if we construct a map on each coordinate chart separately, there is no general way to ensure that the maps coincide where the chart overlaps. Thus in this case we are limited to phase spaces with global coordinates, such as $M = \mathbb{R}^n \times \mathbb{T}^m$. We will point out this restriction where it applies.

If we think of starting with a differential equation $\dot{x} = f$ with a given structure and then constructing maps with the same structure out of f (as is done in numerical integration), the easiest structures are linear symmetries. These are preserved by all Runge–Kutta methods and are discussed in Section 2. The next easiest are linear time-reversing symmetries (Section 3), standard Hamiltonian structure (Section 4) and quadratic first integrals (Section 5). These are preserved by some, but not all, Runge–Kutta methods. The next in line are volume preservation (Section 6) and general first integrals (Section 5). These are in general not preserved by any Runge–Kutta method, but other methods have been discovered, using generating function ideas, for preserving them. Finally, for nonlinear symmetries and nonstandard Hamiltonian structure no general methods at all are known.

2. Systems with symmetries

An ODE $\dot{x} = f(x)$, $x \in \mathbb{R}^n$, has linear symmetry group $G = \{S_i\}$ if

$$S_i f S_i^{-1} = f \tag{10}$$

for all symmetries $S_i \in G$. A generating function form for f satisfying (10) is

$$f = \sum_{S_i \in G} S_i g S_i^{-1}, \tag{11}$$

where the parameter g is any continuous vector field. For maps $x' = \phi(x)$ with linear symmetry group G (i.e., $S_i \phi S_i^{-1} = \phi$ for all $S_i \in G$), any Runge–Kutta method (4), (5) provides a generating function form, where f is given by (11). A more general form for maps, analogous to (11), is given by

$$\phi = \sum_{S_i \in G} S_i \psi S_i^{-1} \tag{12}$$

with parameter $\psi \in C^0(\mathbb{R}^n, \mathbb{R}^n)$.

3. Systems with (symmetries and) time-reversing symmetries

An ODE $\dot{x} = f(x)$, $x \in \mathbb{R}^n$, has linear reversing symmetry group $G = \{S_i\} \cup \{R_i\}$ if

$$S_i f S_i^{-1} = f, \quad R_i f R_i^{-1} = -f \tag{13}$$

for all symmetries $S_i \in G$ and reversing symmetries $R_i \in G$, where each S_i and R_i is a linear diffeomorphism on $\mathbb{R}^n$. A generating function form for f satisfying (13) is

$$f = \sum_{S_i \in G} S_i (g - R g R^{-1}) S_i^{-1}, \tag{14}$$

where R is an arbitrary reversing symmetry in G. (Note that the sum in (14) is only over the symmetries.)

A large class of generating function forms for maps with a linear reversing symmetry group is given by the time-symmetric Runge–Kutta methods:

$$x \mapsto x + \sum_j b_j f(X_j), \qquad X_i = x + \sum_j a_{ij} f(X_j), \qquad a_{\sigma(i),\sigma(j)} + a_{ij} = b_{\sigma(j)} = b_j \tag{15}$$

for some permutation σ of $\{1, \ldots, s\}$, and f is given by (14).

A generating function form for maps with a linear reversing symmetry group $\{S_i\}$ and a (possibly nonlinear) reversing symmetry R is given by the "projection"

$$\chi = \phi R \phi^{-1} R^{-1}, \tag{16}$$

where ϕ is given by (12). For further discussion of these forms and their relationships, see [12]. For methods which preserve arbitrary symmetry groups, not exactly, but to any order for maps near the identity, see [7].

4. Systems with symplectic structure

The form (2) goes over to noncanonical Hamiltonian, or Poisson, systems on a manifold M: given a Poisson 2-vector $J(x)$, we let

$$g : H \to J(x)(\mathrm{d}H) \tag{17}$$

generate the global Poisson vector fields on M [17]. (The g.f.f.'s for canonical maps (e.g. (3)) can extend to Poisson maps in principle [3], but this requires finding local canonical coordinates, which is difficult in general.) Equipped with this form we can write H as a sum and split $g(H)$ into Hamiltonian vector fields:

$$H = \sum_i H_i, \quad g(H_1, \ldots) := g(H) = \sum_i J(x)(\mathrm{d}H_i) \tag{18}$$

(indicating that one can also regard $g(H_1, \ldots)$ as a non-1–1 generating function form). In applications to integrators, the hope is that the constituent systems $\dot{x} = J(x)(\mathrm{d}H_i)$ are simpler than the original one. Either they are integrable, so their flows are computable, or they belong to a simpler class of systems for which generating functions are available. Examples where the flows are computable are:

- canonical systems with separable Hamiltonians, $H = T(p) + V(q)$ [23];
- discretizations of wave equations, $H = L(x) + N(x)$, where L is linear and N is completely local [10];
- N-body systems, $H = \sum_{i,j} F(x_i, x_j)$ where the 2-body system is integrable [26];
- Lie–Poisson systems where each H_i is a function on an abelian subalgebra of the given Lie algebra, such as rigid body systems [22] and the $SU(N)$ truncation of the 2D Euler equations [9];
- the Landau–Lifshitz spin system [2], where a red–black spatial splitting decouples the system.

Because H has been split, properties associated with the specific form of H may be lost, such as energy conservation, symmetries, and integrals (unless they are also properties of each H_i). But all properties associated only with $J(x)$ are preserved: the Casimirs (and hence the symplectic leaves) and symplecticity. In addition, if $\sum_i \partial J_{ij}/\partial x_i = 0$ then the flows are all volume preserving.

Thus this splitting can be useful even if $J(x)$ is not Poisson. Volume and the Casimirs are preserved in any event. Such systems arise when discretizing Hamiltonian PDEs, when the Poisson property is commonly lost [9,15], but skew-symmetry, volume, and some Casimirs can be retained.

We can regard

$$(H_1, \ldots, H_n) \mapsto \exp(J(\mathrm{d}H_1)) \cdots \exp(J(\mathrm{d}H_n)) \tag{19}$$

as a generating function form, if we choose, with parameter space $C^2(M, \mathbb{R}^n)$; but not as a form with parameter $H \in C^2(M, \mathbb{R})$, because it makes little sense to define the splitting independently of H.

5. Systems with an integral

5.1. S-splitting

An ODE $\dot{x} = f(x)$ on a manifold M has an integral I if

$$f(\mathrm{d}I) = 0. \tag{20}$$

Although such f's form a linear space, it is not easy to work in this space directly, so we first seek a generating function form for such systems. Notice that if S is a 2-vector on M, then

$$\dot{x} = S(\mathrm{d}I) \tag{21}$$

has integral I, because $f(\mathrm{d}I) = S(\mathrm{d}I, \mathrm{d}I) = 0$. In fact, (21) generates all such systems [18], for let z be any vector field on M and take

$$S = \frac{2f \wedge z}{z(\mathrm{d}I)} \tag{22}$$

so that in local coordinates,

$$(S(\mathrm{d}I))^i = \sum_j \frac{f^i z^j - f^j z^i}{\sum_k z^k \,\mathrm{d}I_k}\,\mathrm{d}I_j = f^i \tag{23}$$

using (20).

In general, S has singularities on codimension-1 submanifolds of M, giving removable singularities in $S(\mathrm{d}I)$, even though by assumption f is smooth. However, if M has a metric g_{ij}, we have the raising operator $\# : T^*M \to TM$ and can let $z = (\mathrm{d}I)^\#$, or $z^i = \sum_j g^{ij}\,\mathrm{d}I_j$:

$$S = \frac{2f \wedge \mathrm{d}I^\#}{\mathrm{d}I^\#(\mathrm{d}I)}. \tag{24}$$

Then $z(\mathrm{d}I) = \sum_{i,j} \mathrm{d}I_i g^{ij}\,\mathrm{d}I_j$ is only zero where $\mathrm{d}I = 0$, which generically happens only on a set of dimension 0. If these critical points are regular then $f = 0$ there, and the singularity in S is removable. At degenerate critical points, there may be no smooth S for which $f = S(\mathrm{d}I)$, as the example

$$I(x,y) = \frac{1}{2}x^2, \qquad S = \begin{pmatrix} 0 & -1/x \\ 1/x & 0 \end{pmatrix}, \qquad f = \frac{\partial}{\partial y}$$

shows.

Eqs. (22) and (24) give some solutions S to $f = S(\mathrm{d}I)$. To find the general solution for a given f and I, we add any solution of the homogeneous equation $S(\mathrm{d}I) = 0$ to a particular S. These solutions are $S = v \wedge w$ where v and w are any vector fields satisfying $v(\mathrm{d}I) = w(\mathrm{d}I) = 0$. The solution space has dimension $\frac{1}{2}(n-1)(n-2)$. This freedom may be used to find S's with more zero entries, for example. Of course, Hamiltonian or Poisson vector fields with Poisson 2-vector $J(x)$ and Hamiltonian H are already in the form (21), with $S = J$ and $I = H$.

To generate maps with integral I, we hold I constant and split S, i.e., we write S as a sum of 2-vectors:

$$\dot{x} = \sum S_i(\mathrm{d}I). \tag{25}$$

Now, each vector field $S_i(\mathrm{d}I)$ has integral I by construction. In contrast to H-splitting, *every* ODE with an integral (21) can be split into integrable vector fields in this way. On $\mathbb{R}^n$, let S_{ij} be the matrix equal to S in entries (i, j) and (j, i), and zero elsewhere. Each S_{ij}, having rank 2, is automatically Poisson, and we have a two-dimensional Hamiltonian system, which is necessarily integrable.

Because it has been split, any extra structure associated with S (Poisson structure, for example) is in general lost. But in the special case $M = \mathbb{R}^n$, if each $\nabla \cdot S_i = \sum_j \partial S_{i,jk}/\partial x_j = 0$, then each vector field $S_i(\mathrm{d}I)$ is volume preserving, so some volume- and integral-preserving integrators can be constructed in this way. This is particularly relevant for canonical Hamiltonian systems, where

$$S = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$$

is constant, hence splits into two-dimensional volume-preserving pieces. However, not all systems with volume and an integral can be treated in this way – see Section 7.

The flow of each vector field in (25) can now be either
- evaluated exactly, or
- (if only I need be preserved) approximated with an integral-preserving discrete gradient method (see Section 5.2), or
- (if split into 2D systems, and only volume need be preserved) approximated by the area-preserving midpoint rule.

Thus, we can regard the 2D splitting together with one of these methods as a generating function form for maps in each respective class.

Numerically, one advantage of splitting into smaller systems and approximating each by an implicit method is that the implicit equations will be much easier to solve than in a fully implicit method. This will require that $S_i(\mathrm{d}I)$ can be evaluated quickly when $n-2$ of the variables are held fixed.

Good results have been obtained with methods based on S-splitting by Leimkuhler [2] in a study of the Landau–Lifshitz spin system, and by Reich [22] for a particle in a magnetic field. We attribute their good results to volume preservation, and (in the first case) reversibility and energy conservation.

5.2. Discrete gradient method

A second application of the generating function form (21) is described in [5,21]. Like S-splitting, it generates maps with an integral. One replaces the derivative of I by a *discrete gradient* D, approximates $S(x)$ by $\tilde{S}(x,x')$, and uses the map

$$x \mapsto x' = x + \tilde{S}(x,x')DI(x,x'), \tag{26}$$

where D satisfies

$$(x'-x)\cdot DI(x,x') = I(x') - I(x) \tag{27}$$

for all I, x, x'. The general solution of (27) is

$$DI(x,x') = \xi - (x'-x)\frac{\xi\cdot(x'-x) - I(x') + I(x)}{|x'-x|^2}, \tag{28}$$

where $\xi = \xi(x,x') \in \mathbb{R}^n$. Moreover, *every* map with integral I, for every discrete gradient D, can be written in the form (26) for some choice of $\tilde{S}$. Thus, in this case we have complete and roughly parallel generating function forms for both ODEs and maps.

A feature of this construction is its generality: it includes all integral-preserving one-step methods, for example projection methods [25]. The advantage is that this extra freedom can be used to decrease the implicitness or decrease spurious coupling between the degrees of freedom. The task of finding the appropriate choices for $S(x)$, $\tilde{S}(x,x')$, and the discrete gradient in each particular case, may, however, be difficult.

A natural extension of (21) to systems with any number of integrals,

$$\dot{x} = K(\mathrm{d}I_1, \mathrm{d}I_2, \ldots), \tag{29}$$

where K is a multivector, and the corresponding discrete version using discrete gradients, is discussed in [19].

6. Systems preserving volume

On $\mathbb{R}^n$, the flow of the differential equation $\dot{x} = f(x)$ preserves Euclidean volume in phase space if $\nabla \cdot f = 0$. However, this criterion is of little help in determining volume-preserving flows or maps. A generating function form for these systems was given by Feng and Wang [1]; here, we present it on an arbitrary manifold with an arbitrary volume element preserved.

Let μ be a volume element on phase space M (an n-manifold), and let the flow of $\dot{x} = f(x)$ preserve μ. We have

$$0 = \frac{\mathrm{d}}{\mathrm{d}t}(\exp(tf)^*\mu)|_{t=0} = \mathcal{L}_f\mu = i_f\,\mathrm{d}\mu + \mathrm{d}i_f\mu = \mathrm{d}i_f\mu, \tag{30}$$

i.e., $i_f\mu$ must be closed. So we can write

$$i_f\mu = \mathrm{d}\alpha + \gamma, \tag{31}$$

where α is an $n-2$ form and $\gamma \in H^{k-1}(M)$, the $(k-1)$th cohomology of M (the space of $k-1$ forms that are closed but not exact). Moreover, if μ is nondegenerate then (31) determines f as a function of μ, α, and γ. So this g.f.f. is onto. It is not 1–1: we can add any closed $(n-2)$-form to α, or change the representation of γ, without affecting f.

Note the similarity between the form for volume preserving systems and for Hamiltonian systems. If $J(x)$ in (17) is nonsingular, we may write (17) in the form

$$i_f\omega = \mathrm{d}H, \tag{32}$$

where ω is the (closed) 2-form which satisfies $i_J\omega = 1$. (In coordinates, ω is the inverse of J.) The advantage of this formulation is that closed 2-forms ω are easily given, whereas there is no known generating function form for Poisson 2-vectors. Comparing (32) with (31), we see the Hamiltonian (0-form) has been replaced by an $(n-2)$ form, which is not a conserved quantity unless $n = 2$ and $\gamma = 0$. Thus there is no need to distinguish the $\gamma = 0$ case in general, as is done for locally vs. globally Hamiltonian systems.

For the forms of intermediate dimension $2 < k < n$ with $i_f\beta^k = \mathrm{d}\zeta^{k-2}$, the flow of f does preserve the closed k-form β^k, but in general there is no vector field f satisfying this equation for given β^k, ζ^{k-2}.

(We digress to consider a further difference between Hamiltonian and volume preserving systems in this formulation. Let (M, ω) be a symplectic manifold and $H: M \to \mathbb{R}$ the Hamiltonian. If N is a symplectic submanifold of M (i.e., $\omega|_N$ is nondegenerate), then the Hamiltonian dynamics can be constrained to N in a natural way: let $\tilde{\omega} = \omega|_N$ and $\tilde{H} = H|_N$, and $i_{\tilde{f}}\tilde{\omega} = d\tilde{H}$ defines the constrained vector field entirely on N. (This can be shown to agree with various other formulations such as Dirac constraints, variational principles etc. [14].) However, such a restriction is not possible with volume preserving systems, because $\mu|_N = 0$ if $\dim N < \dim M$.

If M has a metric then there is a reasonably natural way out, for then we have the Hodge $*$ isomorphism between k-forms and $(n-k)$-forms. $*\mu$ is a density function on M – it equals 1 for Euclidean volume elements and metrics. *This* function can be restricted, and we can define

$$\tilde{\mu} = *((*\mu)|_N), \quad i_{\tilde{f}}\tilde{\mu} = d\tilde{\alpha} + \tilde{\gamma}. \tag{33}$$

The constrained dynamics determined by $\tilde{f}$ will, however, depend on the metric in general.)

In local coordinates, if $\mu(x) = m(x)\prod \mathrm{d}x_k$ and $\alpha = \sum A_{ij}\prod_{i',j'}\mathrm{d}x_k$, $\gamma = \sum g_j \prod_{j'}\mathrm{d}x_k$ (the primes indicating factors omitted from the product), we have

$$\dot{x}_i = f_i = \frac{1}{m}\left(g_i + \frac{\partial}{\partial x_j}A_{ij}\right), \tag{34}$$

where A is skew, which, apart from the g_i arising from possible non-trivial topology of M, is the form used in [1].

For example, if M is any direct product of copies of $\mathbb{S}^n$, $\mathbb{R}^n$, and $\mathbb{T}^n$, then γ amounts to adding a constant to f in the angular directions corresponding to the $\mathbb{T}^n$.

To get an analogous form for maps, Feng and Wang suggest splitting A into $A = \sum A_{ij}$ where $A_{ij} = A$ in entries (i, j) and (j, i) and is zero elsewhere, and then applying a symplectic method to these two-dimensional Hamiltonian systems. This works in the general case too: the γ term can be split off and treated separately, and the density m gives rise to systems of the form

$$\dot{x}_i = \frac{1}{m}\frac{\partial A_{ij}}{\partial x_j}, \qquad \dot{x}_j = -\frac{1}{m}\frac{\partial A_{ij}}{\partial x_i}. \tag{35}$$

These are Poisson, and hence integrable; in the new time variable $\mathrm{d}\tilde{t} = \mathrm{d}t/m$, they are Hamiltonian. Their flow may not be given in terms of elementary functions, however, in which case the measure-preserving integrator of Quispel [20] may be used.

Of course, such a method is not invariant under the gauge freedom in the choice of A. To get a locally 1–1 g.f.f., we need a family of A's with $(n-1)$ arbitrary functions, which generates all volume preserving ODEs. One such choice, given in [1], is to take A tridiagonal with

$$\frac{\partial A_{i,i+1}}{\partial x_{i+1}} - \frac{\partial A_{i-1,i}}{\partial x_{i-1}} = f_i. \tag{36}$$

That is,

$$\begin{aligned} A_{12} &= \int f_1\,\mathrm{d}x_2 \\ A_{23} &= \int \left(f_2 + \frac{\partial}{\partial x_1}\int f_1\,\mathrm{d}x_2\right)\mathrm{d}x_3 \\ &\ \vdots \end{aligned} \tag{37}$$

(The integrals here are indefinite; any values of the arbitrary constants may be taken. One particular choice is discussed in [1].) To find A from f involves iterated integrals (at least $n/2$-fold) which may be difficult to evaluate. An alternative which avoids this problem is to choose a fixed variable x_k and take $A_{ij} = 0$ for $i, j \neq k$. Then for $i \neq k$,

$$A_{ik} = \int f_i\,\mathrm{d}x_k. \tag{38}$$

In either case the g.f.f. provides a natural splitting into $n-1$ planar measure-preserving systems.

A more complex choice of A, which treats each coordinate equally, is

$$A_{ij} = \frac{1}{n}\left(\int f_i\,\mathrm{d}x_j - \int f_j\,\mathrm{d}x_i\right). \tag{39}$$

Unfortunately, this symmetry is broken when A is split. In this context we mention a result of Feng and Wang [1], which we interpret in this way: if a volume-preserving method is linearly covariant [12] (i.e., changing variables in the ODE commutes with time discretization) then it coincides up to time reparametrization with the exact solution when applied to linear systems. In rough terms, there is no general linearly covariant volume-preserving integrator.

7. Systems preserving volume and an integral

Some flows and maps preserving both volume and an integral were generated in Sections 4 and 5. However, it is clear that all cases could not be covered. The close similarity of (34) and (21) suggests taking on $\mathbb{R}^n$,

$$\dot{x}_i = f_i(x) = \sum_{jk} \frac{\partial}{\partial x_j} \frac{\partial I}{\partial x_k} K_{ijk}(x), \tag{40}$$

where K is a completely skew 3-tensor. Indeed, such vector fields do preserve Euclidean volume and have I as an integral. The question arises, can *all* such vector fields be written in this way?

First, consider systems of the form (40). To generate a map we split K and integrate, or conservatively approximate, the resulting systems. As in Section 6 (volume preserving) and Section 5 (integral preserving), it is always possible to split into integrable systems. For, choose three indices (i, j, k) and let $\widetilde{K}_{i'j'k'} = K_{i'j'k'}$ for (i', j', k') a permutation of (i, j, k), and $\widetilde{K}_{i'j'k'} = 0$ otherwise. Then for $l = i', j', k'$ we have

$$\dot{x}_l = \sum_{m,n} \epsilon_{lmn} \frac{\partial I}{\partial x_m} \frac{\partial K}{\partial x_n} \tag{41}$$

or

$$\dot{x} = \nabla I \times \nabla K, \tag{42}$$

where $K = K_{ijk}$. This is a three-dimensional system preserving volume and the two integrals I and K, and hence it is integrable. It is in fact a Nambu system [16]. One may sum over n, giving a Poisson system with energy I and Casimir K, or sum over m, giving a Poisson system with energy K and Casimir I. It may either be solved by quadratures (perhaps exactly, or to any desired accuracy using numerical Gaussian quadrature) or Poisson integration applied to this second Poisson system (see Section 4) – perhaps by splitting K, which is not an integral of the total system anyway.

Example. Consider the system on $\mathbb{R}^4$ given by

$$\dot{x}_1 = x_2^2 - x_3 x_4^2(1 + x_3), \quad \dot{x}_2 = -x_1 x_2 + x_3 x_4^2, \quad \dot{x}_3 = x_1 - x_2, \quad \dot{x}_4 = x_1 x_4, \tag{43}$$

which is volume preserving and has integral $I = (x_1^2 + x_2^2 + x_3^2 x_4^2)/2$. It may be written in the form (40) with $K_{123} = x_1 + x_2$, $K_{124} = x_2 x_4$, $K_{134} = K_{234} = 0$. This gives the splitting

$$f = f_{123} + f_{124}, \quad f_{123} = \begin{pmatrix} -x_3 x_4^2 \\ x_3 x_4^2 \\ x_1 - x_2 \\ 0 \end{pmatrix}, \quad f_{124} = \begin{pmatrix} x_2^2 - x_3^2 x_4^2 \\ -x_1 x_2 \\ 0 \\ x_1 x_4 \end{pmatrix}, \tag{44}$$

where f_{123} has extra integrals x_4 and K_{123} (and is linear in the planes $x_4 = \text{const.}$), and f_{124} has extra integrals x_3 and K_{124}.

Unfortunately, not all systems preserving volume and an integral can be written in this form (40), because of obstructions depending on the topology of the level sets of the integral I. To see this, we work on a manifold M using differential forms. The representation $f = S(\mathrm{d}I)$ of (21) is not suitable here, so we first find a new representation for vector fields f with an integral I, using $(n-2)$-forms instead of 2-vectors.

First, let α be any $(n-1)$-form. Then $\alpha \wedge dI$ is an n-form, hence proportional to the n-form μ at each point. Suppose $\alpha \wedge \mathrm{d}I = c\mu$. Let $\beta = \alpha/c$. Then

$$i_f\mu = i_f(\beta \wedge \mathrm{d}I) = (i_f\beta) \wedge \mathrm{d}I + (-1)^{n-1}\beta \wedge (i_f\,\mathrm{d}I) = (i_f\beta) \wedge \mathrm{d}I = \theta \wedge \mathrm{d}I, \tag{45}$$

where θ is the $(n-2)$-form $i_f\beta$.

Since the flow of f preserves volume, the right-hand side in (45) must be closed, and

$$\mathrm{d}(\theta \wedge \mathrm{d}I) = \mathrm{d}\theta \wedge \mathrm{d}I, \tag{46}$$

so $\theta|_{I=I_0}$ must be closed. If θ is actually closed in M, and furthermore exact, then we have

$$i_f\mu = \mathrm{d}\zeta \wedge \mathrm{d}I \tag{47}$$

for some $(n-3)$-form ζ, which is the analogue of (40). (If $n=3$, ζ is a 0-form, hence an integral, as in (42).) However, the space of $(n-2)$-forms which are closed on the level set $I = I_0$ depends on the topology of this level set. There is no way to write down the general solution for θ without knowing this topology, which can only be done on a case by case basis. For example, if the level sets are all topologically trivial (e.g. spheres or Euclidean) then (40) does generate all vector fields.

To find a simple example illustrating this point, we take an integral I whose level sets are topologically nontrivial. Let $n=3$ and $I(x,y,z) = x^2+y^2$. The level sets are cylinders (or a line) with $H^1 \cong \mathbb{R}$. Any vector field that winds around the cylinder, such as

$$\dot{x} = y \quad \dot{y} = -x \quad \dot{z} = 1, \tag{48}$$

cannot be written in the form (40). It *can* be written as $\frac{1}{2}(\nabla z + T) \times \nabla I$ where

$$T = \left(y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}\right) \Big/ (x^2+y^2)$$

corresponds to the form θ which is closed but not exact on the cylinders. In this example, every volume preserving vector field preserving I can be written in the form

$$\dot{x} = (\nabla K + g(I)T) \times \nabla I \tag{49}$$

for some functions K and g, but such a form requires knowing the first cohomology group $H^1(\{I = I_0\})$.

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