

Collective symplectic integrators

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Abstract

We construct symplectic integrators for Lie–Poisson systems. The integrators are standard symplectic (partitioned) Runge–Kutta methods. Their phase space is a symplectic vector space equipped with a Hamiltonian action with momentum map J whose range is the target Lie–Poisson manifold, and their Hamiltonian is collective, that is, it is the target Hamiltonian pulled back by J . The method yields, for example, a symplectic midpoint rule expressed in 4 variables for arbitrary Hamiltonians on $\mathfrak{so}(3)^*$. The method specializes in the case that a sufficiently large symmetry group acts on the fibres of J , and generalizes to the case that the vector space carries a bifoliation. Examples involving many classical groups are presented.

Keywords: symplectic integrators, Lie–Poisson systems, reduction

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1. Introduction: symplectic integrators for canonical and noncanonical Hamiltonian systems

A Hamiltonian system on a symplectic manifold is defined by (M, ω, H) where M is a manifold, ω is a symplectic form, and $H: M \rightarrow \mathbb{R}$ is a Hamiltonian; the associated Hamiltonian vector field X_H is defined by $i_{X_H}\omega = dH$, or, in local coordinates z in which $\omega = \frac{1}{2} dz \wedge \Omega dz$, $\dot{z} = X_H(z)$ with $\Omega X_H = \nabla H$. A symplectic integrator for X_H is a one-parameter family of symplectic maps $\varphi_{\Delta t}: M \rightarrow M$ such that $\varphi_0 = id$ and $(\frac{d}{dt}\varphi_t)|_{t=0} = X_H$. Symplectic integrators are known in only a few cases, the main ones being the following [5].

- (i) When (M, ω) is a symplectic vector space, many Runge–Kutta methods are symplectic. The midpoint rule $\varphi_{\Delta t}: z_0 \mapsto z_1$, $\Omega(z_1 - z_0)/\Delta t = \nabla H((z_0 + z_1)/2)$ is an example.

- (ii) When (M, ω) is a symplectic vector space, then given any choice of Darboux coordinates (q, p) on M , many partitioned Runge–Kutta methods are symplectic. (Essentially, because $\omega = dq \wedge dp$ is now linear in q and p , one can apply any Runge–Kutta method to the q component and then determine the p component by symplecticity.)
- (iii) When H can be written as $H = \sum_i H_i$ such that each split vector field X_{H_i} can be integrated exactly, then compositions of their flows provide symplectic integrators.
- (iv) When $M = T^*Q$ with its canonical symplectic form, if the configuration space Q is embedded in a linear space N by constraints (i.e., $Q = \{q \in N : g(q) = 0\}$), then constrained symplectic integrators such as RATTLE are known; the algorithm is expressed in coordinates on the linear space T^*N but is designed in such a way that it induces a symplectic integrator on M .

A Hamiltonian system on a Poisson manifold is defined by $(P, \{, \}, H)$ where P is a manifold, $\{, \}$ is a Poisson bracket, and $H: M \rightarrow \mathbb{R}$ is a Hamiltonian. Poisson maps $\varphi: P \rightarrow P$ are those that preserve the Poisson bracket, i.e., $\{F, G\} \circ \varphi = \{F \circ \varphi, G \circ \varphi\}$ for all $F, G: P \rightarrow \mathbb{R}$. Poisson manifolds are foliated into symplectic leaves, and often these leaves are the level sets of Casimirs, functions C such that $\{C, F\} = 0$ for all F . Consequently, Poisson diffeomorphisms are those that preserve the foliation and pull back the symplectic form on the target leaf to the symplectic form on the source leaf. Hamiltonian vector fields are defined by their action on functions by $\dot{F} = \{F, H\}$. In local coordinates with $\{F, G\} = \nabla F^T K(z) \nabla G$, $X_H(z) = K(z) \nabla H(z)$. The flow of a Hamiltonian vector field is Poisson and, in addition, fixes each leaf. If there are Casimirs, then they are first integrals of X_H for any H . Some main classes of Poisson manifolds are (i) symplectic manifolds (the case that P has a single symplectic leaf); (ii) P a vector space with constant Poisson tensor K ; and (iii) P a vector space with linear Poisson bracket. In this case P is a Lie–Poisson manifold and we have $P = \mathfrak{g}^*$ where $\mathfrak{g}$ is a Lie algebra and $\{F, G\}(z) = z([dF, dG])$ for all $z \in \mathfrak{g}^*$; the symplectic leaves of P are the coadjoint orbits of G in $\mathfrak{g}^*$ and they form important classes of symplectic manifolds.

Symplectic integrators for $(P, \{, \}, H)$ are one-parameter families of Poisson maps $\varphi_{\Delta t}: P \rightarrow P$ such that $\varphi_0 = \text{id}$ and $(\frac{d}{dt}\varphi_t)|_{t=0} = X_H$ and, in addition, fix each leaf. These are only known in a few cases.

- (i) When P is a vector space with constant Poisson bracket, symplectic Runge–Kutta methods are Poisson integrators for any H [15].
- (ii) When $P = \mathfrak{g}^*$ is Lie–Poisson, many Hamiltonians (for example polynomials) can be split into integrable pieces [17].
- (iii) When $P = \mathfrak{g}^*$ is Lie–Poisson, then X_H is the Marsden–Weinstein reduction of a canonical Hamiltonian system on T^*G . Symplectic integrators can be constructed for any H by either (a) constructing a discrete Lagrangian in TG using the exponential map to provide local coordinates on G [1, 14] or (b) embedding G in a linear space and using a constrained symplectic integrator such as RATTLE [18].

However, the integrators from case (iii) are extremely complicated, involving solving implicit equations in Lie groups, infinite series of Lie brackets, and/or using an excessive number of degrees of freedom. For example, to integrate on the two-dimensional sphere, approach (iii)(b) would realize S^2 as a coadjoint orbit in the three-dimensional $\mathfrak{so}(3)^*$, lift to $T^*SO(3)$ (six-dimensional) and embed this in $T^*\mathbb{R}^{3 \times 3}$ (18-dimensional). What is wanted is an approach to constructing symplectic integrators that leads to simple methods, that works for any H , and that uses few extra variables. We achieve this at the price of some extra work beforehand that depends on P .

2. Collective symplectic integrators for Lie–Poisson systems

2.1. Realizations and collective symplectic maps

Definition 1. A *realization* of a Poisson manifold P is a Poisson map $\psi: M \rightarrow P$ where (M, ω) is a symplectic manifold. A realization is *full* if ψ is surjective. If $(M, \omega) = (T^*\mathbb{R}^n, dq \wedge dp)$ then (q, p) are called *canonical* or *Clebsch* variables for P . A function of the form $H \circ \psi: M \rightarrow \mathbb{R}$, where $H: P \rightarrow \mathbb{R}$, is called a *collective Hamiltonian*. A map $\varphi: M \rightarrow M$ is *collective* if there is a map $\tilde{\varphi}: P \rightarrow P$ such that $\tilde{\varphi} \circ \psi = \psi \circ \varphi$. We say the map φ *descends* to $\tilde{\varphi}$ and that $\tilde{\varphi}$ is the *reduced map* of M ; similarly for vector fields.

Note that $\varphi: M \rightarrow M$ is collective if and only if it maps fibres of ψ to fibres of ψ . If φ is collective, the reduced map $\tilde{\varphi}$ is only uniquely defined on the range of M .

Since ψ is a Poisson map, we have $\{F \circ \psi, H \circ \psi\} = \{F, H\} \circ \psi$. The right-hand side is collective, that is, constant on fibres $\psi^{-1}(z)$. The left-hand side is the Lie derivative along $X_{H \circ \psi}$ of the function $F \circ \psi$ that is constant on fibres. Therefore, the flow of $X_{H \circ \psi}$ maps fibres to fibres, or, put another way, is ψ -related to X_H [13]. If ψ is surjective, the vector field $X_{H \circ \psi}$ descends to a vector field on P , namely X_H .

Realizations and collective Hamiltonians are a long-established tool in Hamiltonian dynamics. Key references are [4, 11, 24] and especially [12] which is the main inspiration for our approach. Essentially all of the required geometry is in [12] and our contribution is to find conditions under which that framework can be useful for constructing integrators.

Definition 2. A *collective symplectic integrator* for $(P, \{\cdot, \cdot\}, H)$ is a full realization of P together with a symplectic integrator for $(M, \omega, H \circ \psi)$ that descends to a symplectic integrator for $(P, \{\cdot, \cdot\}, H)$. A *collective symplectic map* for $(P, \{\cdot, \cdot\})$ is a full realization of P together with a symplectic map of (M, ω) that descends to a symplectic (i.e., Poisson and fibre-preserving) map of $(P, \{\cdot, \cdot\})$.

In the most general case, this merely swaps one hard problem (constructing symplectic integrators on P) for three hard problems (finding full realizations, finding fibre-preserving symplectic integrators so that the integrator descends to P , and ensuring that the reduced integrator preserves the symplectic leaves). Note if P has a Casimir C , then $C \circ \psi$ is a first integral of $X_{H \circ \psi}$, but preserving arbitrary integrals of a Hamiltonian system is difficult.

We now let $P = \mathfrak{g}^*$ with its Lie–Poisson structure. An action of a Lie group G on M is said to be (globally) Hamiltonian if it has a momentum map $J: M \rightarrow \mathfrak{g}^*$ that is equivariant with respect to the coadjoint action of G on $\mathfrak{g}^*$, i.e.,

$$J(g \cdot x) = \text{Ad}_{g^{-1}}^* J(x) \quad (1)$$

for all $x \in M, g \in G$ [13]. J is then Poisson and the image $J(M)$ is a union of coadjoint orbits which are the symplectic leaves of $\mathfrak{g}^*$. In this case M is called a *Hamiltonian G -space*. In other words, any Hamiltonian action of G on M provides a realization of $\mathfrak{g}^*$, although it need not be full. Conversely, any Poisson map from M to $\mathfrak{g}^*$ must be the momentum map for some Hamiltonian group action on M [12]. Thus, in the case $P = \mathfrak{g}^*$, we do not lose any generality by restricting attention in our search for realizations to Hamiltonian G -spaces.

The Hamiltonian vector fields of collective Hamiltonians can be calculated in this case using the result of [4] (p 215) that $X_{H \circ J}(x) = \xi_{dH(x)}$ where ξ_p is the infinitesimal generator of the G -action associated with $p \in \mathfrak{g}$; in vector notation,

$$X_{H \circ J}(x) = \Omega^{-1}(TJ(x))^T (\nabla H)(J(x)).$$

According to Weinstein [24], the minimum dimension of a realization of a neighbourhood of $z \in \mathfrak{g}^*$ is equal to $\dim \mathfrak{g} + \dim \mathfrak{g}_z$, which can be as large as $2 \dim \mathfrak{g}$ (by taking $z = 0$). He constructs such a representation, but it is not canonical.

We will present in this section two general approaches to the construction of collective symplectic integrators. The first uses only the basic data M and J and seeks conditions under which a symplectic integrator applied to $X_{H \circ J}$ is collective. We call this the direct approach. The second uses additional structure, a ‘symmetry’ group G_2 that acts on the fibres of J ; we call this the symmetry approach. In section 4 we present examples of both approaches. The direct approach requires a fairly complete understanding of the group orbits and of the fibres of J , and is used in examples 1–3 to provide collective symplectic integrators for $\mathfrak{a}(1)^*$, $\mathfrak{so}(3)^*$ and $\mathfrak{sl}(2)^*$. The symmetry approach is used in examples 4 and 5 to provide collective symplectic integrators for $\mathfrak{o}(n)^*$, $\mathfrak{gl}(n)^*$, and part of $\mathfrak{sp}(2k)^*$.

2.2. The direct approach

Theorem 1. *Let G be a Lie group with a Hamiltonian action on M whose momentum map $J: M \rightarrow \mathfrak{g}^*$ has connected fibres. Let $\varphi: M \rightarrow M$ be a symplectic map.*

- (i) *If φ maps G -orbits to G -orbits then it descends to a map on $J(M) \subset \mathfrak{g}^*$ and that reduced map is (Lie-)Poisson.*
- (ii) *If φ fixes each orbit of G then the reduced map preserves the coadjoint orbits.*

Proof.

- (i) The map φ preserves the orbits of G , so it preserves the distribution tangent to the orbits, $D_x := T(G \cdot x)$. The map φ is symplectic, hence invertible, so $T\varphi|_{D_x}: D_x \rightarrow D_{\varphi(x)}$ is a linear isomorphism. The symplectic orthogonal to D_x is the distribution tangent to the fibres of J and is also preserved by φ , because $\omega(T\varphi.u, T\varphi.v) = \omega(u, v) = 0$ for all $v \in D_x$, $u \in D_x^\perp$, and $T\varphi.D_x = D_{\varphi(x)}$, so $T\varphi.u \in D_{\varphi(x)}^\perp$. Because the fibres of J are assumed to be connected, φ maps fibres of J to fibres of J , that is, it descends to $J(M)$. The reduced map $\tilde{\varphi}$ satisfies $J \circ \varphi = \tilde{\varphi} \circ J$. For all functions F, G on $\mathfrak{g}^*$ we have $\{F, G\} \circ \tilde{\varphi} \circ J = \{F, G\} \circ J \circ \varphi = \{F \circ J, G \circ J\} \circ \varphi = \{F \circ J \circ \varphi, G \circ J \circ \varphi\} = \{F \circ \tilde{\varphi} \circ J, G \circ \tilde{\varphi} \circ J\} = \{F \circ \tilde{\varphi}, G \circ \tilde{\varphi}\} \circ J$ and therefore $\{F, G\} \circ \tilde{\varphi} = \{F \circ \tilde{\varphi}, G \circ \tilde{\varphi}\}$, that is, $\tilde{\varphi}$ is (Lie-)Poisson.
- (ii) If φ fixes each orbit of G then $\varphi(x)$ lies in the orbit $G \cdot x$, that is, $\varphi(x) = g \cdot x$ for some $g \in G$. Therefore from (1), $J(\varphi(x)) = \text{Ad}_{g^{-1}}^* J(x)$ and the reduced map preserves the coadjoint orbits. $\square$

If an integrator φ defines a map from vector fields X to diffeomorphisms $\varphi(X)$, the integrator is said to be G -equivariant if this map is G -equivariant with respect to the action of G on vector fields and on diffeomorphisms, i.e., if $\varphi(Tg.X \circ g) = g^{-1} \circ \varphi(X) \circ g$ for all $g \in G$. For example, all Runge–Kutta methods are affine-equivariant. If the action of G is symplectic, then $Tg.X_H \circ g = X_{H \circ g}$ so in this case $\varphi(X_{H \circ g}) = g^{-1} \circ \varphi(X_H) \circ g$. Our next result shows that equivariance descends to $J(M)$.

Theorem 2. *Let G be a Lie group with Hamiltonian action on M with momentum map J . For a vector field X , we denote by $\varphi(X)$ the corresponding diffeomorphism for the method φ . Assume that φ is a G -equivariant integrator on M such that, for each Hamiltonian H defined on $J(M)$, $\varphi(X_{H \circ J})$ descends on $J(M)$ to a map denoted $\tilde{\varphi}(H)$. Then the map $\tilde{\varphi}$ is equivariant in the sense that $\tilde{\varphi}(H \circ \text{Ad}_{g^{-1}}^*) = \text{Ad}_g^* \circ \tilde{\varphi}(H) \circ \text{Ad}_{g^{-1}}^*$ for any $g \in G$.*

Proof. G acts as a Poisson map, so $X_{H \circ J \circ g} = Tg^{-1}X_{H \circ J} \circ g$ [13, proposition 10.3.2]. Combining the equivariance of φ and the equivariance of J we obtain

$$\varphi(X_{H \circ \text{Ad}_{g^{-1}}^* J}) = g^{-1} \circ \varphi(X_{H \circ J}) \circ g. \quad (2)$$

Now, $\tilde{\varphi}$ is defined by $\tilde{\varphi}(H) \circ J = J \circ \varphi(X_{H \circ J})$. This gives $\tilde{\varphi}(H \circ \text{Ad}_{g^{-1}}^*) \circ J = J \circ \varphi(X_{H \circ \text{Ad}_{g^{-1}}^* \circ J})$. Using (2) and the equivariance of J we finally obtain $\tilde{\varphi}(H \circ \text{Ad}_{g^{-1}}^*) \circ J = \text{Ad}_g^* \circ \tilde{\varphi}(H) \circ \text{Ad}_{g^{-1}}^* \circ J$. We conclude that the result must hold on $J(M)$. $\square$

A consequence is that the reduced integrator will preserve any coadjoint symmetries of H .

Definition 3. Let G act on M . A function $I: M \rightarrow \mathbb{R}^k$ is an invariant of G if $I(g \cdot x) = I(x)$ for all $x \in M$. The function I is a complete invariant of the action of the orbits of G are given by the fibres of I .

Theorem 3. Let G be a Lie group with a Hamiltonian action on M with complete invariant $I: M \rightarrow \mathbb{R}^k$ and whose momentum map $J: M \rightarrow \mathfrak{g}^*$ has connected fibres. Let $\varphi: M \rightarrow M$ be a symplectic map.

- (i) If I is a first integral of φ then the reduced map of φ on $\mathfrak{g}^*$ is (Lie-)Poisson and preserves the coadjoint orbits.
- (ii) If M is a symplectic vector space and I is quadratic then symplectic Runge–Kutta methods applied to $X_{H \circ J}$ are collective symplectic integrators for $(J(M), \{, \}, H)$.
- (iii) If M is a symplectic vector space and there is a Darboux basis in which I is bilinear, then symplectic partitioned Runge–Kutta methods in this basis are collective symplectic integrators for $(J(M), \{, \}, H)$.

Proof.

- (i) By hypothesis, φ preserves I , hence it fixes each group orbit as required by theorem 1.
- (ii) Symplectic Runge–Kutta methods preserve all quadratic first integrals of Hamiltonian systems [5], hence under these hypotheses they fix each group orbit.
- (iii) Partitioned symplectic Runge–Kutta methods preserve all bilinear first integrals of Hamiltonian systems [5], hence under these hypotheses they fix each group orbit. $\square$

If the realization is full then these integrators provide collective symplectic integrators for $(\mathfrak{g}^*, \{, \}, H)$.

The following example shows that Runge–Kutta methods cannot preserve group orbits in general (see figure 1). Let $a \in \mathbb{C}$ and let $G = \mathbb{R}^{>0}$ act on $M = \mathbb{C}$ by $t \cdot z = e^{at} z$; consider any vector field tangent to the orbits. When a is imaginary, the orbits are the origin and the circles $|z|^2 = \text{const.}$ and are fixed by symplectic Runge–Kutta methods. When a is real, the orbits are the origin and the straight open rays meeting the origin. This action has no smooth invariants (the orbit closures intersect at 0, so any continuous invariant must be constant). Each line through the origin is invariant, and is invariant under all Runge–Kutta methods; each contains an invariant open ray, which is preserved by ‘positivity-preserving’ Runge–Kutta methods. When a is neither real nor imaginary, the orbits are spirals; there are no smooth invariants and the orbits are not fixed by any Runge–Kutta method. Thus, the proposed integration method can only cope with fairly simple actions. This example motivates the following extension of theorem 3.

A *polyhedral set* is the intersection of affine subspaces and closed half-subspaces. An example is the orthant $x_i \geq 0$ for all i . Sufficient conditions for a Runge–Kutta method to preserve this orthant for sufficiently small time steps when it is invariant are known [7]; such methods are called *positivity-preserving*. The midpoint rule is positivity-preserving; positivity is preserved for time steps less than $2/L$ where L is the Lipschitz constant of the vector field.

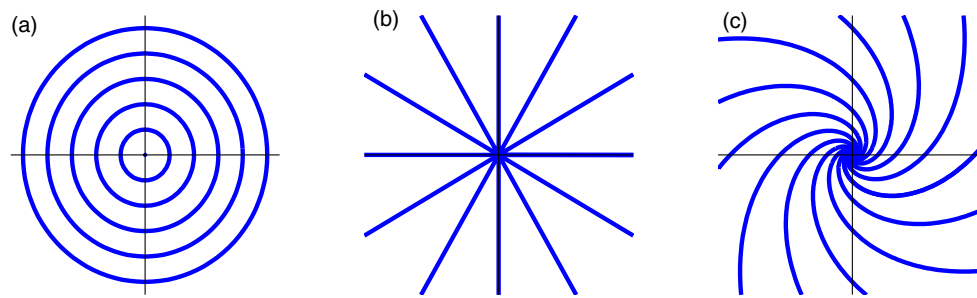


Figure 1. Can standard integrators preserve orbits of linear actions? Orbits of the action $t \cdot z = e^{at}z$ of $\mathbb{R}^{>0}$ on $\mathbb{C}$ are shown for $a = i$, $a = 1$, and $a = 1 + i$. (a) When $a \in i\mathbb{R}$, the orbits are the level sets of the quadratic $|z|^2$, and are preserved by the midpoint rule $z_{n+1} = z_n + \Delta t f((z_n + z_{n+1})/2)$ when f is any smooth vector field tangent to the circles. (b) When $a \in \mathbb{R}$, the orbits are rays. Although the *lines* through the origin are preserved by any Runge–Kutta method for any vector field tangent to the rays, the *rays* are preserved only by ‘positivity-preserving’ Runge–Kutta methods, for sufficiently small time steps. (c) When a is neither real nor imaginary, the orbits are spirals, and are typically not preserved by any Runge–Kutta method.

Theorem 4. Let G be a Lie group with a Hamiltonian action on the symplectic vector space M whose momentum map $J: M \rightarrow \mathfrak{g}^*$ has connected fibres and which has quadratic (respectively, bilinear) invariants $I: M \rightarrow \mathbb{R}^k$ such that the closure of each orbit is the intersection of an invariant polyhedral set and a fibre of I . Then for sufficiently small time steps, positivity-preserving symplectic Runge–Kutta methods applied to $X_{H \circ J}$ are collective symplectic integrators for $(J(M), \{\cdot, \cdot\}, H)$.

Proof. Positivity-preserving Runge–Kutta methods preserve also preserve invariant polyhedral sets for sufficiently small time steps [7]. Quadratic invariants are preserved by symplectic Runge–Kutta methods. Therefore, the closure of each orbit is fixed by the given methods. The boundary of an orbit closure is itself, by hypothesis, the intersection of an invariant polyhedral set and a fibre of I and hence is itself invariant. Since the map is invertible, the interior of the orbit closure is also invariant. This is either an orbit (in which case we are done) or a union of orbits (in which case the argument is repeated). Thus every orbit is fixed by the method and theorem 1 gives the result. $\square$

If the orbit closures are just slightly more general, for example the intersection of a polyhedral set and a fibre of an invariant quadratic, then a positivity-preserving symplectic Runge–Kutta method need not fix them. (In $\mathbb{R}^3$, the circle $x_1 = 0$, $\|x\|^2 = 1$ in the flow of $\dot{x} = J(x)x$, $J^T = -J$, $J_{1k} = f_k(x_1, \|x\|^2 - 1)$, $f(0, 0) = 0$ is such a set.)

2.3. The symmetry approach

Often there is a second group acting on the fibres of J . If its orbits are large enough, and respected by the integrator, this can be enough to ensure that the integrator is collective.

Theorem 5. Let G_1 be a group with a Hamiltonian action on M and momentum map J_1 . Let G_2 be a group acting on M that fixes each fibre of J_1 and is transitive on them. Then any G_2 -equivariant symplectic map is collective.

Proof. By transitivity, any two points on the fibre $J_1^{-1}(z)$ may be written in the form $x, g_2 \cdot x$ for some $g_2 \in G_2$. Then G_2 -equivariance gives $\varphi(g_2 \cdot x) = g_2 \cdot \varphi(x)$, that is, $\varphi(g_2 \cdot x)$ lies on the G_2 -orbit ($= J_1$ -fibre) of $\varphi(x)$. Thus the J_1 -fibres map to J_1 -fibres and the map descends; from equivariance of J_1 it is collective. $\square$

Consider $G = GL(1)$ acting by cotangent lifts on $T^*\mathbb{R}$ with momentum map $J = qp$. G acts on the fibres of J , and is transitive on generic fibres, but is not transitive on $J^{-1}(0)$. However, we shall see that its orbits are still large enough to construct collective integrators. This motivates the following definition.

Definition 4. A smooth function $\Psi: M \rightarrow P$ has complete symmetry group G if G acts smoothly on M , has invariant Ψ , and there are no non-constant G -invariant continuous functions on any fibre of Ψ .

If Ψ is a complete invariant for G , i.e., if the fibres of Ψ are the orbits of G , then G is a complete symmetry group for Ψ . If the action of G is transitive on a dense subset of each fibre of Ψ , then G is a complete symmetry group for Ψ . If the orbits of G are closed (in particular if the action of G is proper, which happens if G is compact), then the property of being a complete symmetry group is equivalent to transitivity of the action of G on the fibres.

Lemma 1. Let $\Psi: M \rightarrow P$ have complete symmetry group G . Then any continuous map $\varphi: M \rightarrow M$ which maps orbits of G to orbits of G is Ψ -collective.

Proof. Let $x \in \Psi(M)$ and consider one fibre $L := \Psi^{-1}(x)$. Let $N := \Psi^{-1}(\Psi(\varphi(L)))$ be the set of fibres of Ψ in $\varphi(L)$, and quotient this space by the fibres to obtain N/Ψ . Consider a continuous function $g: N/\Psi \rightarrow \mathbb{R}$. Pulling back g by Ψ gives a continuous function h on N which is constant on the orbits of G . Therefore $h|_L$ is also constant on the orbits of G . Because G is a complete symmetry group of Ψ , $h|_L$ must be constant. The function g must then be constant, because of the definition of N . Since N/Ψ is Hausdorff (because the fibres are closed subsets of M), and all its continuous functions are constant, it must reduce to one point, that is, N consists of exactly one fibre. We conclude that φ maps fibres of Ψ to fibres of Ψ , that is, φ is Ψ -collective. $\square$

For example, if G_1 has a Hamiltonian action on M and momentum map J_1 with complete symmetry group G_2 , then any G_2 -equivariant symplectic map is collective. Our main example of this situation is the following.

Theorem 6. Let G_1 be a group with a Hamiltonian action on M and momentum map J_1 with complete symmetry group G_2 that has momentum map J_2 . Let H be a Hamiltonian on $\mathfrak{g}_1^*$.

- (i) If the action of G_2 is linear then symplectic Runge–Kutta methods applied to $X_{H \circ J_1}$ are collective symplectic integrators for $(J_1(M), \{, \}, H)$.
- (ii) If the action of G_2 is a linear cotangent lift then symplectic partitioned Runge–Kutta methods applied to $X_{H \circ J_1}$ are collective symplectic integrators for $(J_1(M), \{, \}, H)$.

Proof. First note that $H \circ J_1$ is constant on fibres of J_1 , hence G_2 -invariant.

- (i) The linear symmetry G_2 of $X_{H \circ J_1}$ is preserved by symplectic Runge–Kutta methods. Lemma 1 now gives the result.
- (ii) The linear cotangent lift symmetry G_2 of $X_{H \circ J_1}$ is preserved by symplectic partitioned Runge–Kutta methods. Lemma 1 now gives the result. $\square$

Often there is a complete symmetry group G_2 that makes (G_1, G_2) into a dual pair.

Definition 5. A C^k dual pair is a pair G_1, G_2 of Lie groups with Hamiltonian actions on M and momentum maps J_1, J_2 such that the C^k functions that commute with J_1 -collective functions are C^k -collective for J_2 and vice versa. That is, $\{f, J_1\} = 0, f \in C^k(M) \Rightarrow f \in J_2^* C^k(J_2(M))$. Analytic dual pairs are defined analogously.

For a dual pair, the orbits of G_1 are contained in the fibres of J_2 and the orbits of G_2 are contained in the fibres of J_1 . The Hamiltonian vector field $X_{F \circ J_1}$ is G_2 -equivariant and the Hamiltonian vector field $X_{F \circ J_2}$ is G_1 -invariant.

Note that if f is constant on G_2 -orbits, then $\langle df, X_{J_2} \rangle = 0 = \{f, J_2\}$, so the dual pair condition ensures that f is J_1 -collective. That is, G_2 is a complete symmetry group for J_1 , so G_2 -equivariant symplectic integrators are collective.

Theorem 7. Let G_1, G_2 be a C^k or analytic dual pair acting on $M = \mathbb{R}^n$ and let $H: M \rightarrow \mathbb{R}$ be a smooth Hamiltonian. If the action of G_2 is linear (cotangent lift) then (partitioned) symplectic Runge–Kutta methods produce collective symplectic integrators that descend to C^{k-1} or analytic symplectic integrators on $(J_1(M), \{, \}, H)$.

Proof. The integrator preserves J_2 . Differentiation with respect to the time-step h represents the integrator as the time- h flow of a nonautonomous Hamiltonian vector field on M ; let $\tilde{H}(x, t)$ be the Hamiltonian. Because its flow preserves J_2 , $\{\tilde{H}, J_2\} = 0$. The dual pair condition implies that $\tilde{H} = \hat{H} \circ J_1$, where $\hat{H}$ is C^k or analytic; thus its flow, the reduced integrator, is C^{k-1} or analytic. $\square$

Definition 5 is an instance of Weinstein's definition [24] of dual pair, which involves two Poisson maps ψ_i from M to Poisson manifolds P_i . There are many other versions and refinements of the concept of dual pair; see [9, 10, 22]. One that is of use in constructing integrators for classical Lie–Poisson manifolds is the original representation-theoretic dual pair of Howe [8], two subgroups G_1, G_2 of $Sp(M)$ such that G_1 (respectively G_2) is the centralizer of G_2 (respectively G_1). When the G_i are reductive (i.e., when every G_i -invariant subspace of M has a G_i -invariant complement, $i = 1, 2$), the quadratic functions J_2 form a generating set for the G_1 -invariant polynomials. If H is any polynomial that satisfies $\{H, J_1\} = 0$, then $H = \hat{H}(J_2)$ where $\hat{H}$ is a polynomial. That is, one has a ‘first fundamental theorem’—a set of polynomials that generate all polynomial invariants—for reductive Howe dual pairs [8, 9]. Consequently, these (G_1, G_2) form analytic dual pairs:

Theorem 8. Let (G_1, G_2) be subgroups of $Sp(M)$ such that J_1 (resp. J_2) forms a generating set for the G_2 (resp. G_1)-invariant polynomials on M and such that J_1 (resp. J_2) is surjective. Then (G_1, G_2) forms an analytic dual pair.

Proof. Let H be analytic and such that $\{H, J_1\} = 0$. Expand $H = \sum_k H_k$ in a Taylor series where H_k is homogeneous of degree k . Then $\{H_k, J_1\}$ is homogeneous of degree k and thus $\{H_k, J_1\} = 0$. By assumption, there are polynomials $\hat{H}_k: \mathfrak{g}_2^* \rightarrow \mathbb{R}$ such that $H_k = \hat{H}_k \circ J_2$. Because H is analytic, $\sum H_k(x) = \sum (\hat{H}_k \circ J_2)(x)$ is convergent, hence $\hat{H} := \sum \hat{H}_k$ is convergent at $J_2(x)$. Since J_2 is surjective, $\hat{H}$ is analytic on $\mathfrak{g}_2^*$. $\square$

3. Collective integrators from bifoliations

We have seen that we can construct symplectic integrators on Poisson manifolds from standard symplectic integrators in some cases from a Hamiltonian group action (theorems 1, 3, 4) and from two commuting Hamiltonian group actions (theorem 7). Theorem 7 is a special case of

theorem 1, but it gives a little more, namely, it specifies the invariants that need to be preserved, it provides Poisson integrators for two spaces (corresponding to the two groups), and it relates the construction to the standard examples of Howe dual pairs. One can ask if it is possible, instead, to generalize theorem 1, being prepared, of course, to get a little less in return. The key structures are the foliations defined by the orbits and by the fibres of the momentum map (in theorem 1) or the fibres of each momentum map (in theorem 7). These generalize to a *bifoliation*, a structure discussed in [2, 11, 23] whose properties we summarize briefly here.

Let $\mathcal{F}$ be a foliation of a symplectic manifold (M, ω) . The polar of $\mathcal{F}$, if it exists, is the unique foliation $\mathcal{F}^\perp$ of M such that the tangent spaces of its leaves are the symplectic orthogonals of the tangent spaces of the leaves of $\mathcal{F}$. The leaves of $\mathcal{F}$ and of $\mathcal{F}^\perp$ have dimensions that sum to the dimension of M ; their intersection can be nontrivial. A foliation which has a polar is called *symplectically complete*, and $(\mathcal{F}, \mathcal{F}^\perp)$ is called a *bifoliation* of M . A foliation is symplectically complete iff the Poisson bracket of any two functions that are constant on leaves is again constant on leaves. In the case that $M/\mathcal{F}$ is a manifold, $\mathcal{F}$ is symplectically complete iff there is a Poisson structure on $M/\mathcal{F}$ such that the projection map $\psi: M \rightarrow M/\mathcal{F}$ is Poisson; such a structure is unique [2].

Theorem 9. *Let $(\mathcal{F}, \mathcal{F}^\perp)$ be a bifoliation of the symplectic manifold (M, ω) such that $M/\mathcal{F}$ is a manifold. Let $\psi: M \rightarrow M/\mathcal{F}$ be the projection and let $H: M/\mathcal{F} \rightarrow \mathbb{R}$. Then $X_{H \circ \psi}$ fixes each leaf of $\mathcal{F}^\perp$ and any symplectic integrator for $H \circ \psi$ that fixes each leaf of $\mathcal{F}^\perp$ descends to a symplectic integrator of X_H in the Poisson manifold $M/\mathcal{F}$. In particular, when M is a symplectic vector space and $\mathcal{F}^\perp$ is the set of fibres of a set of quadratic functions, then symplectic Runge–Kutta methods applied to $X_{H \circ \psi}$ descend to symplectic integrators of X_H .*

Proof. Any symplectic map that preserves $\mathcal{F}$ (respectively, $\mathcal{F}^\perp$) necessarily preserves $\mathcal{F}^\perp$ (respectively $\mathcal{F}$) and hence descends to a Poisson map on $M/\mathcal{F}$ and on $M/\mathcal{F}^\perp$. The crucial step is to ensure that the reduced map on $M/\mathcal{F}$ fixes each coadjoint orbit. This follows from proposition 14.21 of [11] which states that the image under ψ of a leaf of $\mathcal{F}^\perp$ is contained in a symplectic leaf of $M/\mathcal{F}$. Thus, any symplectic map that fixes each leaf of $\mathcal{F}^\perp$ must fix each coadjoint orbit in $M/\mathcal{F}$. $\square$

Theorem 9 is the most general case; however, it gives somewhat less than the previous theorems because the Poisson manifold is constructed in a somewhat convoluted way from the quadratic functions and the projection ψ is defined abstractly. In practice one will also need the leaves of $\mathcal{F}$ to be the fibres of functions that can be used to define ψ .

There is a special case of theorem 9 which is particularly nice and which produces minimum-dimensional realizations and minimum-dimensional collective symplectic integrators. It uses the following construction of Nekhoroshev [20]; see also [2]. Let $f_1, \dots, f_k$ be k commuting functions on (M, ω) . Then their fibres are coisotropic and symplectically complete. Their polar is isotropic and their projection to the quotient of M by the polar lie in its symplectic leaves. In particular, if $(f_1, \dots, f_{2n-k}) : M \rightarrow \mathbb{R}^{2n-k}$ is a submersion and

$$\{f_i, f_j\} = 0, \quad i = 1, \dots, k, \quad j = 1, \dots, 2n - k$$

then the f_i define a bifoliation with $\mathcal{F}$ the fibres of $f_1, \dots, f_{2n-k}$ isotropic; $\mathcal{F}^\perp$ the fibres of $f_1, \dots, f_k$ coisotropic; and $f_1, \dots, f_k$ the lifts of the Casimirs of the Poisson manifold $M/\mathcal{F}$, whose symplectic leaves have dimension $2n - 2k$. Moreover, we may take $f_1, \dots, f_{2n-k}$ as local coordinates on $M/\mathcal{F}$. In our application, $f_1, \dots, f_k$ should be quadratic. Moreover, we can even drop the ‘collective’ and consider any Hamiltonian with first integrals f_i :

Theorem 10. *Let M be a symplectic vector space and let $f_1, \dots, f_k$ be k commuting quadratic functions on M . Then their Hamiltonian vector fields X_{f_i} are integrable and generate an*

abelian group action (with momentum map $f_1, \dots, f_k$) whose orbits form the isotropic foliation $\mathcal{F}$ polar to the fibres of $f_1, \dots, f_k$. Symplectic Runge–Kutta methods applied to Hamiltonians with first integrals $f_1, \dots, f_k$ (i.e., such that $\{H, f_i\} = 0$ for $i = 1, \dots, k$) descend to symplectic integrators on the Poisson manifold $M/\mathcal{F}$. If $\mathcal{F}$ is the set of fibres of the functions $f = (f_1, \dots, f_{2n-k})$ then symplectic Runge–Kutta methods applied to $H \circ f$ form collective symplectic integrators.

4. Examples

The examples are arranged in order of increasing dimension, starting with the two-dimensional nonabelian Lie algebra. Recall that all cotangent lifted actions, and all linear symplectic actions, are Hamiltonian [13]. We use momentum maps that are Poisson for the ‘+’ Lie–Poisson bracket; the ‘−’ bracket can be obtained by changing the sign of the momentum map.

Example 1. (a) Let $G = A(1)$, the group of affine transformations of $\mathbb{R}$, the smallest nonabelian Lie group. Let G act on $M = T^*\mathbb{R}$ by cotangent lifts, i.e., $(a, b) \cdot (q, p) = (aq + b, p/a)$, $a, b \in \mathbb{R}$. Then $J(q, p) = (qp, p)$. Let (w_1, w_2) be coordinates on $\mathfrak{g}^*$. There is a two-dimensional coadjoint orbit $\{(w_1, w_2): w_2 \neq 0\}$ and many zero-dimensional coadjoint orbits, $\{(w_1, 0)\}$ for each w_1 . The fibres of J consist of the q -axis and the points off the q -axis; they are connected. $J(M)$ is not quite all of $\mathfrak{g}^*$: it consists of the origin together with the two half-planes. The vector field $X_{H \circ J}$ is

$$\begin{aligned}\dot{q} &= q \frac{\partial H}{\partial w_1}(qp, p) + \frac{\partial H}{\partial w_2}(qp, p) \\ \dot{p} &= -p \frac{\partial H}{\partial w_1}(qp, p)\end{aligned}$$

which is the generator of the group action corresponding to ∇H . Any partitioned symplectic Runge–Kutta method that fixes the group orbits (the q -axis and its complement) will, from theorem 1(ii), provide a collective symplectic integrator for $J(M)$. The orbit closures are the polyhedral sets $\{(q, p): p \geq 0\}$, $\{(q, p): p \leq 0\}$, and $\{(q, 0)\}$, and thus from theorem 4, the midpoint rule fixes the group orbits for sufficiently small time steps.

(b) An action of G for which $J(M) = \mathfrak{g}^*$ can be constructed by prolonging the above action to act diagonally on $T^*\mathbb{R}^2$. The momentum map $J(q, p) = (p \cdot q, p_1 + p_2)$ is surjective and has connected fibres. There are two bilinear invariants, $I_1 := (q_2 - q_1)p_1$ and $I_2 := (q_2 - q_1)p_2$, which classify generic orbits, and which are preserved by partitioned symplectic Runge–Kutta methods. However, the fibre with $I_1 = I_2 = 0$ is three-dimensional and contains several orbits,

$$\begin{aligned}&\{(q_1, q_1, p_1, p_2): q_1 \in \mathbb{R}, p_2/p_1 = \text{const.}\}, \\ &\{(q_1, q_2, 0, 0): q_1 \neq q_2\}, \text{ and} \\ &\{(q_1, q_1, 0, 0): q_1 \in \mathbb{R}\}.\end{aligned}$$

Their closures are polyhedral sets, so from theorem 4 the midpoint rule is a collective symplectic integrators for $(\mathfrak{g}^*, \{\cdot, \cdot\}, H)$.

Example 2. (a) Let $G_1 = O(3)$ with its natural cotangent lifted action on $M = T^*\mathbb{R}^3$. Its momentum map $J_1 = q \times p$ is surjective. The fibre of J_1 through (q, p) is $\{(aq + bp, cq + dp): ad - bc = 1\}$, which is connected. The invariants of G_1 are generated by $(q \cdot q, p \cdot p, q \cdot p)$

which are quadratic and form a complete set of invariants. Therefore symplectic Runge–Kutta methods such as the midpoint rule applied to $X_{H \circ J_1}$, namely

$$\begin{aligned}\dot{q} &= -q \times \nabla H(q \times p) \\ \dot{p} &= -p \times \nabla H(q \times p),\end{aligned}$$

generate Lie–Poisson integrators on $\mathfrak{o}(3)^*$ for any H . The lifted coadjoint orbits are $\|q \times p\|^2 = \text{const.}$, which are quartic invariants of $X_{H \circ J_1}$. However, from theorem 1, we know that they are conserved by the integrator.

The Hamiltonian vector fields of the invariants suggest that J_1 has a complete symmetry group $G_2 = SL(2)$ with $J_2 = (q \cdot q, p \cdot p, q \cdot p)$, and linear action

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \cdot (q, p) = (aq + bp, cq + dp)$$

which is the natural action of $SL(2)$ on $(T^*\mathbb{R})^3$. The lifted Casimir

$$\|q \times p\|^2 = \|J_1(q, p)\|^2 = (q \cdot q)(p \cdot p) - (q \cdot p)^2$$

is collective for J_2 —another way of seeing why it is conserved by the integrator.

(b) (See figure 2.) It is interesting to ‘dualize’ this example by considering Hamiltonians $H \circ J_2$. These are $O(3)$ -invariant Hamiltonians such as classical central-force Hamiltonians $\|p\|^2/2 + V(\|q\|^2)$. The invariants of G_2 are $J_1(q, p) = q \times p$ which are bilinear. The action of G_1 is transitive on the fibres of J_2 so we can use the symmetry group approach. The action of G_1 is a linear cotangent lift, hence from theorem 5 partitioned symplectic Runge–Kutta methods, such as leapfrog, yield collective integrators for $J_2(M) \subset \mathfrak{sl}(2)^*$ on $J_2(M)$. Note J_2 is not surjective. The Casimir in $\mathfrak{sl}(2)^* \ni w$ is $C := w_1 w_2 - w_3^2$ and $C \circ J_2 = \|q \times p\|^2 \geq 0$, so $J_2(M) = \{w \in \mathfrak{sl}(2)^* : w_1 \geq 0, w_2 \geq 0, C \geq 0\}$ which is a solid cone. Figure 2 shows some orbits of Hamiltonian systems on $\mathfrak{sl}(2)^*$ (and the coadjoint orbits they inhabit) calculated using the collective leapfrog method.

Example 2(b) is closely related to the symplectic reduction of $O(3)$ -invariant Hamiltonians $H \circ J_2$. Indeed, all $O(3)$ - (and all $SO(3)$ -) invariant Hamiltonians are collective for J_2 . Most treatments of reduction for this example (see, e.g., [13]) do not involve $\mathfrak{sl}(2)^*$, the dual of the algebra of invariants, instead passing to a symplectic reduced space with coordinates $(\|p\|^2, q \cdot p)$ or $(\|q\|, \|p\|)$. See [10] for a treatment that features the algebra of invariants. A feature of the $\mathfrak{sl}(2)^*$ approach is that it allows one to see the relationship between orbits of different angular momentum and to visualize the orbits as intersections of energy and Casimir level sets.

Example 3 (Hopf-fibration realization of $\mathfrak{so}(3)^*$). For $\mathfrak{so}(3)^*$, the leaves are the origin (with three-dimensional isotropy) and the 2-spheres $\|z\| = \text{const.}$ (with one-dimensional isotropy) so the minimum possible dimension to cover a sphere is 4. There is a canonical four-dimensional realization, not just of the neighbourhood of a sphere, but of all of $\mathfrak{so}(3)^*$. Let $G_1 = SU(2)$ with its natural action on $M = \mathbb{C}^2$ which is canonical for $(z_1, z_2) = (q_1 + ip_1, q_2 + ip_2) \in M$. The momentum map $J: M \rightarrow \mathfrak{su}(2)^* \cong \mathfrak{so}(3)^* \cong \mathbb{C} \times \mathbb{R} \in (w_1 + iw_2, w_3)$ is given by $J(z_1, z_2) = (\frac{1}{2}\bar{z}_1 z_2, \frac{1}{4}(|z_1|^2 - |z_2|^2))$ and is surjective with connected fibres (circles and points $e^{i\alpha}(z_1, z_2)$.) Hamilton’s equations for $H \circ J_1$ are

$$\begin{aligned}\dot{z}_1 &= -\frac{1}{2} \left(iz_2 \frac{\partial H}{\partial w_1} + z_2 \frac{\partial H}{\partial w_2} + iz_1 \frac{\partial H}{\partial w_3} \right) \\ \dot{z}_2 &= \frac{1}{2} \left(-iz_1 \frac{\partial H}{\partial w_1} + z_1 \frac{\partial H}{\partial w_2} + iz_2 \frac{\partial H}{\partial w_3} \right)\end{aligned}$$

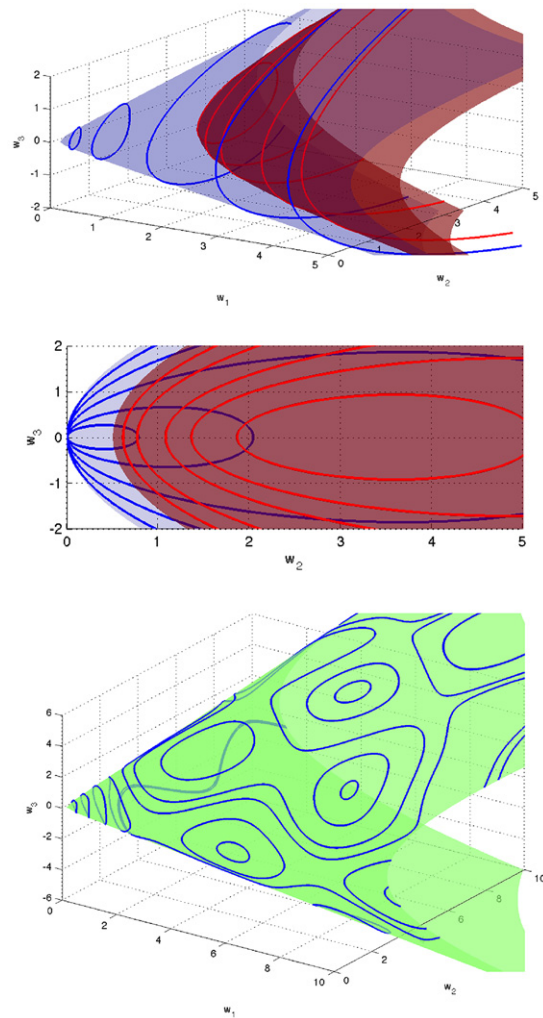


Figure 2. Some orbits of Hamiltonian systems on $\mathfrak{sl}(2)^*$ and the coadjoint orbits they inhabit. The coadjoint orbits are given by $w_1 w_2 - w_3^2 = C$; the cone $C = 0$ and hyperboloid $C = 2.5$ are shown. Top: Hamiltonian $H(w_1, w_2, w_3) = w_1 + \frac{1}{2} w_1^2 + \frac{1}{2} w_2$. The collective Hamiltonian for $J = (q \cdot q, p \cdot p, q \cdot p)$ is $H \circ J = \|q\|^2 + \frac{1}{2} \|q\|^4 + \frac{1}{2} \|p\|^2$. Calculated with the collective leapfrog method with $\Delta t = 0.01$. Middle: as before, showing the ‘standard’ reduced variables w_2, w_3 . Bottom: Hamiltonian $\sum_{i=1}^3 \cos w_i$ on $C = 0$. The intersection of the energy and Casimir level sets creates a complex phase portrait.

The only independent invariant of G_1 is $I := |z_1|^2 + |z_2|^2$ and it is quadratic and a complete invariant. Therefore from theorem 3(ii) symplectic Runge–Kutta methods applied to $H \circ J_1$ produce symplectic integrators for $\mathfrak{so}(3)^*$.

Some examples are shown in figures 3–6. We first illustrate the resulting collective midpoint rule for the free rigid body in figure 3. In figure 4 we apply the collective Gauss Runge–Kutta methods to the same system, confirming that the energy errors of the s -stage method are $\mathcal{O}((\Delta t)^{2s})$, as expected, and do not grow in time, and that the Casimir errors are of

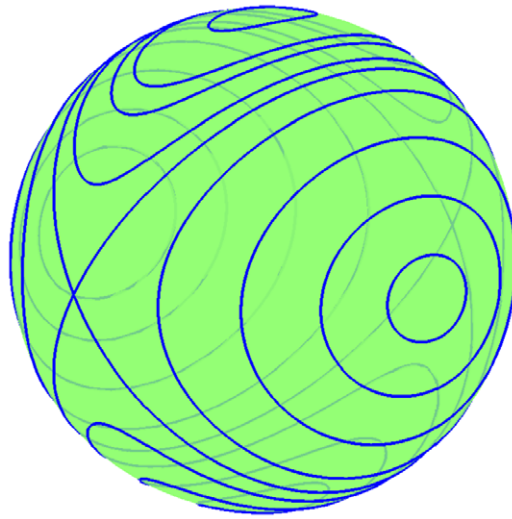


Figure 3. Some orbits of the rigid body Hamiltonian $H = \frac{1}{2}w_1^2 + \frac{1}{4}w_2^2 + \frac{5}{3}w_3^2$ calculated using the four-dimensional Hopf-fibration realization of $\mathfrak{so}(3)^*$ with the collective midpoint rule and time step 0.04.

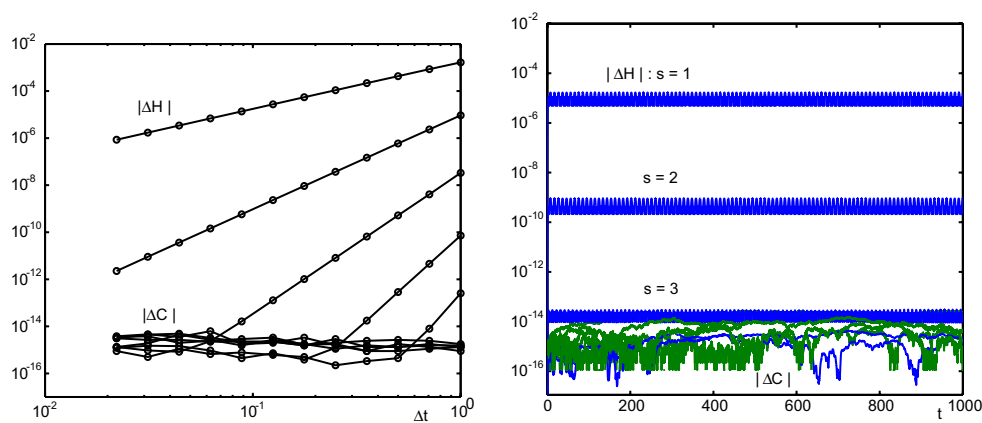


Figure 4. For the ODE in in figure 3, illustrating the behaviour of Gauss Runge–Kutta methods with $s = 1$ –5 stages, orders 2–10. The errors in the Casimir $C = \|w\|^2$ are at roundoff and the errors in the Hamiltonian do not grow. Left: integration time $t = 20$, varying Δt ; right: $\Delta t = 0.1$, varying t .

the order of roundoff error. Figure 5 illustrates the phase portrait obtained when applying the collective midpoint rule to the nonseparable Hamiltonian $\prod_{i=1}^3 \sin 4w_i$ and time step 0.01; the implementation is simple, as only the vector field needs to be specified, and the resulting phase portrait agrees with the exact phase portrait to the accuracy shown. Finally, a small, time-periodic forcing is applied to this system and the resulting 1-period map is shown in figure 6. The orbit forms a ‘chaotic web’, a typical phenomenon in two-dimensional area-preserving dynamics.

Another application of these integrators is to generate smooth symplectic integrators for Hamiltonian systems on S^2 equipped with the Euclidean area form: extend the Hamiltonian