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Momentum conserving symplectic integrators *

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Abstract

In this paper, we show that symplectic partitioned Runge–Kutta methods conserve momentum maps corresponding to linear symmetry groups acting on the phase space of Hamiltonian differential equations by extended point transformation. We also generalize this result to constrained systems and show how this conservation property relates to the symplectic integration of Lie–Poisson systems on certain submanifolds of the general matrix group GL(n).

1. Introduction

We are concerned in this paper with differential equations

$$\begin{aligned} q' &= f(q,p), \\ p' &= g(q,p), \end{aligned} \qquad (1)$$

where $q, p \in \mathbb{R}^n$. We assume that (1) has a first integral of the form

$$q^t W p = \text{const.}, \qquad (2)$$

where W is a constant $n \times n$ matrix; i.e.

$$f^t(q,p)\, Wp + q^t W g(q,p) = 0 \qquad (3)$$

for all $(q,p) \in \mathbb{R}^n \times \mathbb{R}^n$.

We will frequently consider the case that (1) has been derived from an Hamiltonian $H : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$; i.e.

$$f(q,p) = \nabla_p H(q,p)$$

and

$$g(q,p) = -\nabla_q H(q,p)\,.$$

First integrals of the form (2) arise, for example, in the context of Hamiltonians which are invariant under a matrix group G acting on the phase space $\mathbb{R}^n \times \mathbb{R}^n$ by extended point transformation [11,13]. In this case, the first integral is given by the momentum map corresponding to the group action [11,13]. A typical example is provided by the action of the SO(3) on $\mathbb{R}^3 \times \mathbb{R}^3$ with angular momentum as the corresponding momentum map.

In this paper we derive necessary conditions for partitioned Runge–Kutta (PRK) method to conserve first integrals of the form (1). It turns out that these are exactly the same conditions which make a PRK method a symplectic integrator when applied to Hamiltonian differential equations (see Sanz-Serna [16] for an overview on symplectic methods). This corresponds to a similar result, given by Cooper [3], for non-partitioned Runge–Kutta methods. The conservation

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of angular momentum by explicit symplectic Runge–Kutta–Nyström methods has been discussed before by Zhang and Skeel [18].

We also consider constrained Hamiltonian systems

$$\begin{aligned} q' &= \nabla_p H(q,p)\,, \\ p' &= -\nabla_q H(q,p) - \nabla_q g(q)\lambda\,, \\ 0 &= g(q)\,, \end{aligned} \tag{4}$$

and show that a similar result holds for the symplectic constraint-preserving PRK methods introduced by Jay [8] and Reich [14]. Based on this, we provide an elementary construction of symplectic integrators for Lie–Poisson systems associated to subgroups of the general matrix group GL(n). This provides an alternative to the construction given by Ge and Marsden [5], Ge [4], and Channell and Scovel [2]. In contrast to our approach, their construction, although more general, is based on the generating function method and on a coordinatization of the group. Applications of our results include multibody dynamics, the free rigid body, the heavy top, and Zeitlin's truncation [19] of the Euler fluid equations.

During the final stage of this work we discovered that, independently of us, a similar approach to the symplectic integration of Lie–Poisson systems has recently been given by McLachlan and Scovel [12].

2. Partitioned Runge–Kutta methods

The discretization of the differential equation (1) by a partitioned Runge–Kutta (PRK) method with Butcher's tableaux [6]

$$\begin{array}{cc} c & A \\ & b^t \end{array} \qquad \begin{array}{cc} \hat{c} & \hat{A} \\ & \hat{b}^t \end{array}$$

leads to the system

$$q_{n+1} = q_n + h\sum_{i=1}^{s} b_i f(Q^i,P^i)\,,$$

$$p_{n+1} = p_n + h\sum_{i=1}^{s} \hat{b}_i g(Q^i,P^i)\,,$$

$$Q^i = q_n + h\sum_{j=1}^{s} a_{ij} f(Q^i,P^i) \quad (i=1,\dots,s)\,,$$

$$P^i = p_n + h\sum_{j=1}^{s} \hat{a}_{ij} g(Q^i,P^i) \quad (i=1,\dots,s)\,.$$

It is convenient to express these equations in a more compact form using tensor product notation. The tensor product $T\otimes S$, of an arbitrary $p\times q$ matrix T and an arbitrary $r\times m$ matrix S, is defined by

$$T\otimes S = \begin{pmatrix} t_{11}S & t_{12}S & \dots & t_{1q}S \\ t_{21}S & t_{22}S & \dots & t_{2q}S \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ t_{p1}S & t_{p2}S & \dots & t_{pq}S \end{pmatrix}.$$

An account of the properties of tensor products is given by Lancaster [9]. Using this notion, a PRK method is given by the equations

$$\begin{aligned} q_{n+1} &= q_n + (b^t\otimes I)F\,, \\ p_{n+1} &= p_n + (\hat{b}^t\otimes I)G\,, \\ Q &= e\otimes q_n + (A\otimes I)F\,, \\ P &= e\otimes p_n + (\hat{A}\otimes I)G\,, \end{aligned} \tag{5}$$

where $e^t = [1,1,\dots,1]$, I is the identity matrix, and

$$Q = \begin{pmatrix} Q^1 \\ Q^2 \\ \cdot \\ \cdot \\ \cdot \\ Q^s \end{pmatrix}, \qquad F = h\begin{pmatrix} f(Q^1,P^1) \\ f(Q^2,P^2) \\ \cdot \\ \cdot \\ \cdot \\ f(Q^s,P^s) \end{pmatrix},$$

etc.

Theorem 2.1. A partitioned Runge–Kutta method conserves quadratic first integrals of the form (2) if

$$B\hat{A} + A^t\hat{B} - b\hat{b}^t = 0 \tag{6}$$

and

$$\hat{b} = b, \tag{7}$$

where B ($\hat{B}$) is the diagonal matrix given by $Be = b$ ($\hat{B}e = \hat{b}$).

Proof. We follow here the proof by Cooper [3] for Runge–Kutta methods. The first two equations in (5) give

$$q_{n+1}^t W p_{n+1} - q_n^t W p_n = q_n^t(\hat{b}^t \otimes W)G + F^t(b \otimes W)p_n + F^t(b\hat{b}^t \otimes W)G.$$

Using now the equations for the stage variables Q and P in (5) and the fact that B and $\hat{B}$ are symmetric, we obtain

$$Q^t(\hat{B} \otimes W)G = q_n^t(\hat{b}^t \otimes W)G + F^t(A^t\hat{B} \otimes W)G$$

and

$$F^t(B \otimes W)P = F^t(b \otimes W)p_n + F^t(B\hat{A} \otimes W)G.$$

These results may be combined to yield

$$q_{n+1}^t W p_{n+1} - q_n^t W p_n = -F^t[(B\hat{A} + A^t\hat{B} - b\hat{b}^t) \otimes W]G + \hat{B} \otimes Q^t W G + B \otimes F^t W P$$

with the right side equal to zero if the conditions (6), (7) and (3) hold. □

Remark 2.1. If (1) is a Hamiltonian differential equation, then a PRK method, satisfying the conditions (6) and (7), conserves also the symplectic structure of the phase space [16].

3. Hamiltonian systems with symmetries

Let G be a Lie subgroup of the general matrix Lie group $GL(n)$ of $\mathbb{R}^n$ [13]. We let G act on $\mathbb{R}^n$ by matrix multiplication on the left; i.e.

$$q \mapsto Tq,$$

where $T \in G$ is the corresponding matrix in $\mathbb{R}^{n\times n}$. The induced extended point transformation on $\mathbb{R}^n \times \mathbb{R}^n$ is given by

$$\begin{pmatrix} q \\ p \end{pmatrix} \mapsto \begin{pmatrix} Tq \\ T^{-t}p \end{pmatrix}, \tag{8}$$

Corresponding to this transformation there is a momentum map $J_L(q,p)$ (where subscript L indicates that G acts on the left) [1,11]. Furthermore, if the Hamiltonian H is invariant under the extended point transformation of G on $\mathbb{R}^n \times \mathbb{R}^n$; i.e.,

$$H(q,p) = H(Tq, T^{-t}p) \tag{9}$$

for all $T \in G$, then the corresponding momentum map $J_L(q,p)$ is a first integral of the differential Eq. (1).

Example 3.1. Let SO(3) act on $q \in \mathbb{R}^3$ by matrix multiplication. Then the corresponding momentum map is given by

$$J_L(q,p) = q \times p,$$

which, of course, is the standard formula for the angular momentum [1]. A Hamiltonian H is invariant under the extended point transformation of SO(3) on $(q,p) \in \mathbb{R}^3 \times \mathbb{R}^3$ if H is of the form $H(|q|, q^t p, |p|)$.

Since the components J_L^i $(i = 1, \ldots, n)$ of the momentum map J_L are of type

$$J_L^i(q,p) = q^t W^i p,$$

where W^i is a proper $n \times n$ matrix, Theorem 2.1 and Remark 2.1 immediately yield the following.

Theorem 3.1. Assume that the Hamiltonian H, generating the differential equation (1), is invariant under the extended point transformation of G on $\mathbb{R}^n \times \mathbb{R}^n$; i.e., assume that (9) holds for all linear transformations $T \in G$. Then a PRK method (5) is symplectic and conserves the corresponding momentum map $J_L(q,p)$, if the method satisfies the conditions (6) and (7).

Remark 3.1. An alternative proof of Theorem 3.1 is possible: For symplectic algorithms preservation of momentum up to a constant follows from the equivariance of the algorithm with respect to the corresponding symmetry group [4]. Now PRK methods are equivariant with respect to the extended point transformation (8) which implies the preservation of the corresponding momentum map up to a constant. If the algorithm has a fixed point, then the momentum map is conserved exactly. Note that the above theorem does not need this additional assumption.

4. Constrained Hamiltonian systems

In this section, we consider constrained Hamiltonian systems (4) with H and g invariant under the extended point transformation of G on $\mathbb{R}^n \times \mathbb{R}^n$; i.e.

$$H(q,p) = H(Tq, T^{-t}p)$$

and

$$g(q) = g(Tq)$$

for all $T \in G$. Here $g : \mathbb{R}^n \to \mathbb{R}^m$, $m < n$, is a vector valued function. We denote its derivative by $g_q(q) \in \mathbb{R}^{n\times m}$ and use the notation $\nabla_q g(q) = g_q^t(q) \in \mathbb{R}^{m\times n}$.

Upon introducing the canonical Poisson bracket

$$\{F,G\} = F_q \nabla_p G - F_p \nabla_q G,$$

$F, G : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$, we can rewrite (4) as

$$\begin{aligned} q' &= \{q, H\}, \\ p' &= \{p, H\} + \{p, g\}\lambda, \\ 0 &= g. \end{aligned} \tag{10}$$

Since $g = 0$, we obtain

$$\begin{aligned} 0 &= g' \\ &= \{g, H\} \end{aligned}$$

as a hidden constraint. Hence the phase space $\mathcal{M}$ of the constrained system (4) is defined by

$$\mathcal{M} = \{(q,p) : g(q) = 0,\ g_q(q)\nabla_p H(q,p) = 0\}.$$

and the configuration space $\mathcal{N}$ by

$$\mathcal{N} = \{q : g(q) = 0\}.$$

The symplectic structure on $\mathcal{M}$ is given by the restriction of the canonical symplectic structure on $\mathbb{R}^{2n}$ to $\mathcal{M}$ [11]. If the Hamiltonian H is of the form

$$H(q,p) = \tfrac{1}{2}(p^t M(q)^{-1} p) + V(q),$$

where $M(q)$ is a positive definite matrix, then

$$\mathcal{M} = \{(q,p) : g(q) = 0,\ g_q(q) M(q)^{-1} p = 0\}$$

can be identified with $T^*\mathcal{N}$ through the inner product

$$\langle x, y\rangle_q = x^t M(q) y,$$

$x, y \in T_q\mathbb{R}^n$, as a metric on $T\mathbb{R}^n$ (see McLachlan and Scovel [12] for a discussion of the general case).

Discretization of (4) by a PRK method results in a system of equations similar to (5) except that G is now given by

$$G = h \begin{pmatrix} -\nabla_q H(Q^1, P^1) - \nabla_q g(Q^1)\Lambda^1 \\ -\nabla_q H(Q^2, P^2) - \nabla_q g(Q^2)\Lambda^2 \\ \cdot \\ \cdot \\ \cdot \\ -\nabla_q H(Q^s, P^s) - \nabla_q g(Q^s)\Lambda^s \end{pmatrix}. \tag{11}$$

and that we have to add the constraints $0 = g(Q^i)$, $i = 1, \ldots, s$. In the context of constrained Hamiltonian systems, PRK methods that satisfy $q_{n+1} = Q^s$ are of special interest. As shown by Jay [8] and Reich [14], one can find symplectic PRK with this property and, furthermore, by a proper choice of Λ^s, these methods also satisfy the hidden constraint exactly. Hence, such methods conserve the phase space $\mathcal{M}$; i.e. $(q_n, p_n) \in \mathcal{M}$ for all $n \geq 1$.

It is straightforward to verify the following generalization of Theorem 3.1 to constrained systems:

Theorem 4.1. Assume that the Hamiltonian H and the constraint function g, generating the constrained system (4), are invariant under the extended point transformation of G on $\mathbb{R}^n \times \mathbb{R}^n$. Then a PRK method applied to the system (4) is symplectic and conserve the corresponding momentum map $J_L(q,p)$, if the corresponding Butcher's tableaux satisfy the conditions (6) and (7).

Proof. The symplecticity of the scheme, i.e. the preservation of the symplectic structure on $\mathcal{M}$, has been proven in [8,14]. The momentum map J_L is again linear in (q,p) and each component J_L^i can be written as

$$J_L^i(q,p) = q^t W^i p.$$

Furthermore, since H and g are invariant under the extended point transformation, each J_L^i satisfies

$$0 = H_p(q,p)\, W^i p - q^t W^i \nabla_q H(q,p)$$

and

$$0 = q^t W^i \nabla_q g(q)$$

for all (q, p). Thus, provided (7) holds, the discretized equations satisfy

$$0 = \hat{B} \otimes Q^t WG + B \otimes F^t WP ,$$

independently of the values of Λ^i in (11) and the proof of Theorem 2.1 also applies to the discretization of the constrained formulation (4). □

Example 4.1. In [14], Reich gave the following first-order symplectic integrator:

$$\begin{aligned} q_{n+1} &= q_n + h\nabla_p H(q_n, P) , \\ P &= p_n - h\nabla_q H(q_n, P) - h\nabla_q g(q_n)\Lambda , \\ 0 &= g(q_{n+1}) , \\ p_{n+1} &= P - h\nabla_q g(q_{n+1})\mu , \\ 0 &= g_q(q_{n+1})\nabla_p H(q_{n+1}, p_{n+1}) , \end{aligned}$$

which can be written as a PRK method. Hence, this scheme also conserves the momentum map J_L.

5. Reduction and Lie–Poisson integrators

Let $\mathrm{GL} = \mathrm{GL}(n) \subset \mathbb{R}^{n\times n}$ denote the general matrix group of $\mathbb{R}^n$ and let $\mathfrak{gl} = \mathbb{R}^{n\times n}$ be the corresponding Lie algebra. Upon introducing the inner product

$$\langle x, y\rangle = \mathrm{tr}\,(xy^t)$$

on $\mathfrak{gl}$, we can pull back the canonical symplectic structure on $T^*\mathrm{GL}$ to $T\mathrm{GL}$. Here tr denotes the trace operator. Thus we can do, as before, Hamiltonian mechanics on the tangent bundle $T\mathrm{GL}$ [11]. Note that q and p are now matrix valued quantities. Furthermore, due to the definition of the inner product, $\nabla_q H(q,p) \in \mathbb{R}^{n\times n}$ and $\nabla_p H(q,p) \in \mathbb{R}^{n\times n}$ are defined by

$$dH(q,p) = \langle \nabla_q H(q,p), dq\rangle + \langle \nabla_p H(q,p), dp\rangle .$$

We let GL act on itself by left translation. The induced extended point transformation on $T\mathrm{GL}$ is again given by (8). We denote the corresponding momentum maps by $J_L : T\mathrm{GL} \to \mathfrak{gl}$, $J_L(q,p) = pq^t$, and $J_R : T\mathrm{GL} \to \mathfrak{gl}$, $J_R(q,p) = q^t p$ (J_R is the momentum map corresponding to the action of GL on itself by right translation). If the Hamiltonian H is invariant under the extended point transformation on the left, then there is a well-known reduction from $T\mathrm{GL}$ to $\mathfrak{gl}$ given by the momentum map J_R (see Arnold [1], Marsden and Ratiu [11], or Olver [13] for an overview on this subject). The equations of motion on $\mathfrak{gl}$ are given by the reduced Hamiltonian on $\mathfrak{gl}$ and by the corresponding Lie–Poisson structure on $\mathfrak{gl}$ which is defined in the following way [11,13]: Let F_L, G_L be two functions on $\mathfrak{gl} = T_{id}\mathrm{GL}$ and let $\{\,,\,\}$ denote the canonical Poisson bracket on $T\mathrm{GL}$. Then the reduced Lie–Poisson bracket $\{\,,\,\}_-$ on $\mathfrak{gl}$ is given by [11]

$$\begin{aligned} &\{F_L, G_L\}_-\,(\Pi) \\ &\quad = \{F_L \circ J_R, G_L \circ J_R\}\,(q = I, p = \Pi) \end{aligned} \tag{12}$$

and the reduced equation of motion on $\mathfrak{gl}$ becomes

$$\Pi' = \{\Pi, H_L\}_- ,$$

where $H_L(\Pi) = H(I, \Pi)$ and $\Pi = J_R(q,p)$. Since

$$\Pi' = (q')^t p + q^t p'$$

and

$$\begin{aligned} q' &= \nabla_p H(q,p) , \\ p' &= -\nabla_q H(q,p) , \end{aligned}$$

the reduced equation of motion is equivalent to

$$\Pi' = (\nabla_p H(I, \Pi))^t \Pi - \nabla_q H(I, \Pi) .$$

Special integrators for Hamiltonian systems on $\mathfrak{gl}^*$, $\mathfrak{gl}$, respectively (and also for Hamiltonian systems on sub-algebras of $\mathfrak{gl}^*$, $\mathfrak{gl}$, respectively), that conserve the Lie–Poisson structure have been derived by Ge and Marsden [5], Channell and Scovel [2], and Ge [4]. These schemes are based on the generating function method and require a coordinatization of the group under consideration. Here we show how symplectic PRK methods for constrained Hamiltonian systems on $T\mathrm{GL}$ are related to Lie–Poisson integrators on the corresponding reduced phase space. Independently of us, a similar approach has recently been taken by McLachlan and Scovel [12].

Let G be a Lie subgroup of GL. Let us assume that (at least locally around the identity matrix I) G can be given by an implicit system of equations

$$G=\{q\in GL: g(q)=0\}.$$

Example 5.1. If $G=\mathrm{SO}(n)$, then the constraint function g is given by $g(q)=q^tq-I$.

Let us consider now Hamiltonian functions H on $T\,\mathrm{GL}$ that are invariant under the extended point transformation of G on $T\,\mathrm{GL}$. By imposing the constraint $q\in G$, the corresponding equations of motion are given by the constrained formulation

$$\begin{aligned} q' &= \nabla_pH)(q,p\,, \\ p' &= -\nabla_qH(q,p)-\nabla_qg(q)\lambda\,, \\ 0 &= g(q)\,, \end{aligned} \tag{13}$$

with the corresponding configuration space

$$\begin{aligned}\mathcal{M}=\{(q,p)\in TGL: g(q) \\ =0,\ g_q(q)\,\nabla_pH(q,p)=0\}.\end{aligned}$$

Here $g:\mathbb{R}^{n\times n}\to\mathbb{R}^m$, $\lambda\in\mathbb{R}^m$, and $\nabla_qg(q)\lambda$ is defined by $\nabla_qg(q)\lambda=\sum\lambda_i\nabla_qg_i(q)$, where ∇_qg_i denotes the gradient of the ith component of the vector valued constraint function g.

Before looking at the discretization of these equations, let us formulate the equations of motion of the corresponding reduced system on $\mathfrak{gl}$. First note that

$$J_R(\mathcal{M})=\mathcal{M}_I\,,$$

with $\mathcal{M}_I\subset\mathfrak{gl}$ given by

$$\mathcal{M}_I=\{\Pi\in\mathfrak{gl}:\ g_q(I)\,\nabla_pH(I,\Pi)=0\}.$$

To see this, apply the extended point transformation to the constraint equation

$$0=g_q(q)\,\nabla_pH(q,p)$$

to obtain

$$0=g_q(Tq)\,TT^{-1}\,\nabla_pH(Tq,T^{-t}p)\,.$$

With $T=q^{-1}$, this yields

$$\begin{aligned}0&=g_q(I)\,\nabla_pH(I,q^tp)\\ &=g_q(I)\,\nabla_pH(I,\Pi)\,.\end{aligned}$$

Hence, $\mathcal{M}_I\subset\mathfrak{gl}$ is the reduced phase space of the constrained Hamiltonian system (13). Let us now introduce the reduced Hamiltonian $H_L:\mathfrak{gl}\to\mathbb{R}$ by

$$H(q,p)=H_L\circ J_R\ (q,p)$$

for all $(q,p)\in\mathcal{M}$. As for the unconstrained case (see Marsden and Ratiu [11]), the reduced equations in the variable $\Pi=J_R(q,p)\in\mathfrak{gl}$ are obtained from (13) by

$$\Pi'=\{J_R,H_L\circ J_R\}+\{J_R,g\}\lambda\,,$$

where we used the formulation (10) and replaced p by J_R and H by $H_L\circ J_R$. By restricting $\{J_R,H_L\circ J_R\}$ to $\mathfrak{gl}$ and using the Lie–Poisson bracket (12), this can be rewritten as

$$\Pi'=\{\Pi,H_L\}_- - q^t\,\nabla_qg(q)\lambda\,.$$

Hence, since

$$q^t\,\nabla_qg(q)=\nabla_qg(I)$$

and $\Pi\in\mathcal{M}_I$, we obtain the reduced equations

$$\begin{aligned}\Pi' &= \{\Pi,H_L\}_- - \nabla_qg(I)\lambda\,, \\ 0 &= g_q(I)\nabla_pH(I,\Pi)\,,\end{aligned} \tag{14}$$

Following the discussion in [12], one can also show that the corresponding reduced equation on the Lie algebra $\mathfrak{g}\subset\mathfrak{gl}$ of G is simply given by

$$\begin{aligned}\Pi'&=\{\Pi,H_L\}_- - \nabla_qg(I)\lambda\,,\\ 0&=g_q(I)\Pi\,,\end{aligned}$$

i.e., the orthogonal projection of $\mathfrak{gl}$ onto $\mathfrak{g}$ restricted to $\mathcal{M}_I$ is an isomorphism between the two Lie algebras $\mathfrak{g}$ and $\mathcal{M}_I$.

Remark 5.1. There is an interesting relation of (14) to the Euler equation for ideal incompressible fluids [11]. If we formally replace the finite dimensional group GL by the infinite dimensional diffeomorphism group and $\mathfrak{gl}$ by the infinite dimensional Lie algebra of vector fields on a given manifold M, then the Euler equation

$$v' = -\nabla_v v + \operatorname{grad} p\,,$$
$$0 = \operatorname{div} v\,,$$

can be considered as a special case of (14). Here $\mathfrak{g}$ is the infinite dimensional Lie algebra of divergence free vector fields and G is the group of volume preserving diffeomorphism. Note that the Euler equation is obtained by right reduction [11], i.e., we would have to replace H_L by H_R, which for the Euler equation is given by

$$H_R(v) = \tfrac{1}{2} \int_M |v|^2 \mu\,,$$

and $\{\,,\,\}_-$ by the corresponding $\{\,,\,\}_+$ on the dual of the Lie algebra of all vector fields on M. Note that

$$\{v, H_R(v)\}_+ = -\nabla_v v\,.$$

Furthermore, we formally have $g_q(I) = \operatorname{div}$, $\operatorname{grad} = (\operatorname{div})^t$, and the pressure p plays the role of the multiplier λ in (14). Thus the reduced phase space is $\mathcal{M}_I = \mathfrak{g}$ the space of divergence free vector fields on M. The Euler equation for rigid bodies will be discussed in Example 5.3 below.

Let us now return to the discretization of (13). If these equations are discretized by a symplectic PRK method that preserves the constraints exactly, we get a symplectic transformation $S : \mathcal{M} \to \mathcal{M}$ that conserves the momentum map J_L; i.e.

$$J_L \circ S = J_L\,.$$

Thus, by the Arnold–Marsden–Weinstein reduction [1,4,11], we can define a Poisson transformation on $\mathcal{M}_I$, $S_0 : \mathcal{M}_I \to \mathcal{M}_I$, by

$$S_0\,(\Pi) := J_R \circ S\ (q = I, p = \Pi)$$

(Note that $J_R(\mathcal{M}) = \mathcal{M}_I$.)

Theorem 5.1. The integration scheme, defined by

$$\Pi_{n+1} = S_0\,(\Pi_n)\,,$$

provides a Lie–Poisson integrator for the Hamiltonian equations (14) on the reduced phase space $\mathcal{M}_I$. The order of the scheme is the same as the order of S. Furthermore, since S conserves the momentum map J_L, S_0 conserves the coadjoint orbits [11] of (14).

Proof. Since S and J_R are Poisson maps, S_0 is obviously a Poisson map too. For initial conditions $(q(0), p(0)) = (I, \Pi(0))$, the solutions of (13) and (14) are related by $\Pi(t) = J_R(q(t), p(t))$, thus S_0 has the same order as S. □

Example 5.2. A first-order Lie–Poisson integrator can be obtained by using the scheme discussed in Example 4.1. In this case, we would have to take $(q_n = I, p_n = \Pi_n)$ and use the resulting (q_{n+1}, p_{n+1}) to obtain $\Pi_{n+1} = q_{n+1}^t p_{n+1}$.

Example 5.3. As an application we consider the Euler equation for rigid bodies [1]. Here GL = GL(3) and $G = \mathrm{SO}(3)$. The constraint function g is given by

$$g(q) = q^t q - I\,.$$

Let us consider a quadratic Hamiltonian

$$H(q,p) = \tfrac{1}{2}\operatorname{tr}(pJ^{-1}p^t)\,,$$

where tr is the trace operator and $J \in \mathrm{GL}(3)$ is a positive definite matrix. For simplicity we assume from now on that J has entries only in the main diagonal. Note that H is invariant under the extended point transformation of the O(3) on $T\,\mathrm{GL}(3)$.

The equations of motion of the corresponding constraint system are given by

$$\begin{aligned} q' &= p\,J^{-1}\,,\\ p' &= -2q\lambda\,,\\ 0 &= q^t q - I\,, \end{aligned} \qquad (15)$$

where λ is a symmetric 3×3 matrix.

Let us now reduce these equations to $\mathfrak{gl}(3)$. The reduced Hamiltonian H_L is simply given by $H_L(\Pi) = H(\Pi)$ and the corresponding reduced equation can be obtained by differentiating $\Pi = q^t p$ with respect to time; i.e.

$$\begin{aligned} \Pi' &= (q')^t p + q^t p' \\ &= J^{-1}\Pi^t\Pi - 2\lambda \end{aligned}$$

A further differentiation of the constraint $\Pi \in \mathfrak{so}(3)$; i.e.,

$$0 = \Pi + \Pi^t$$

with respect to time yields

$$\lambda = \tfrac{1}{4}(J^{-1}\Pi^t\Pi + \Pi^t\Pi J^{-1})$$

and we obtain the reduced equation

$$\Pi' = \tfrac{1}{2}(J^{-1}\Pi^t\Pi - \Pi^t\Pi J^{-1}),$$

which, upon introduction of the matrix commutator $[A, B] = AB - BA$, $A, B \in \mathfrak{gl}$, can be rewritten as

$$\Pi' = \tfrac{1}{2}[\Pi, J^{-1}\Pi + \Pi J^{-1}].$$

Note that $(J^{-1}\Pi + \Pi J^{-1}) \in \mathfrak{so}(3)$. Using now the standard isomorphism between $\mathbb{R}^3$ and $\mathfrak{so}(3)$, we identify Π with $x \in \mathbb{R}^3$ and $\frac{1}{2}(\Pi J^{-1} + J^{-1}\Pi)$ with $M^{-1}x$ where M is a matrix with entries in the main diagonal only and

$$(M^{-1})_{ii} = \tfrac{1}{2}\sum_{i \neq j}(J^{-1})_{jj}.$$

Thus we finally obtain the standard Euler equation for rigid bodies in $\mathbb{R}^3$; i.e.

$$x' = x \times M^{-1}x, \qquad (16)$$

where M is the inertial tensor of the rigid body and x the body angular momentum. The Hamiltonian is the kinetic energy of the body; i.e.

$$H(x) = \tfrac{1}{2}x^t M^{-1}x.$$

As pointed out, e.g. by Reich [15], the Euler equation (16) can be integrated numerically by rewriting (16) as the sum of three Hamiltonian vector fields $X_i = x \times \nabla H_i(x)$ where $H_i(x) = \frac{1}{2}x_i^2(M^{-1})_{ii}$. Each of these vector fields is linear in x and can be solved exactly. By applying the Baker–Campbell–Hausdorff formula [17], one can show that the scheme

$$S_0(x) = \exp(hX_1) \circ \exp(hX_2) \circ \exp(hX_3)\,(x)$$

is of first order in the step-size h and naturally preserves the Lie–Poisson structure of the Euler equation. Of course, one could obtain another Lie–Poisson integrator by applying the first order scheme, as described in Example 4.1, to the constraint system (15) and then reducing the resulting scheme to the $\mathfrak{so}(3)$ as suggested in this section. In this case we would obtain

$$Q = I + hPJ^{-1},$$
$$P = \Pi_n - 2h\lambda,$$
$$0 = Q^tQ - I,$$

and

$$\Pi_{n+1} = Q^t(P - 2h\mu),$$
$$0 = \Pi_{n+1} + \Pi_{n+1}^t.$$

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