Hamilton-Pontryagin Integrators on Lie Groups

Thesis by
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Abstract

In this thesis structure-preserving time integrators for mechanical systems whose configuration space is a Lie Group are derived from a Hamilton-Pontryagin (HP) variational principle. In addition to its attractive properties for degenerate mechanical systems, the HP viewpoint also affords a practical way to design discrete Lagrangians, which are the cornerstone of variational integration theory. The HP principle states that a mechanical system traverses a path that extremizes an HP action integral. The integrand of the HP action integral consists of two terms: the Lagrangian and a kinematic constraint paired with a Lagrange multiplier (the momentum). The kinematic constraint relates the velocity of the mechanical system to a curve on the tangent bundle. This form of the action integral makes it amenable to discretization.

In particular, our strategy is to implement an s-stage Runge-Kutta-Munthe-Kaas (RKMK) discretization of the kinematic constraint. We are motivated by the fact that the theory, order conditions, and implementation of such methods are mature. In analogy with the continuous system, the discrete HP action sum consists of two parts: a weighted sum of the Lagrangian using the weights from the Butcher tableau of the RKMK scheme, and a pairing between a discrete Lagrange multiplier (the discrete momentum) and the discretized kinematic constraint. In the vector space context, it is shown that this strategy yields a well-known class of symplectic partitioned Runge-Kutta methods including the Lobatto IIIA-IIIB

pair which generalize to higher-order accuracy.

In the Lie group context, the strategy yields an interesting and novel family of variational partitioned Runge-Kutta methods. Specifically, for mechanical systems on Lie groups we analyze the ideal context of EP systems. For such systems the HP principle can be transformed from the Pontryagin bundle to a reduced space. To set up the discrete theory, a continuous reduced HP principle is also analyzed. It is this reduced HP principle that we apply our discretization strategy to. The resulting integrator describes an update scheme on the reduced space. As in RKMK we parametrize the Lie group using coordinate charts whose model space is the Lie algebra and that approximate the exponential map. Since the Lie group is non abelian, the structure of these integrators is not the same as in the vector space context.

We carry out an in-depth study of the simplest integrators within this family that we call variational Euler integrators; specifically we analyze the integrator's efficiency, global error, and geometric properties. Because of their variational character, the variational Euler integrators preserve a discrete momentum map and symplectic form. Moreover, since the update on the configuration space is explicit, the configuration updates exhibit no drift from the Lie group. We also prove that the global error of these methods is second order. Numerical experiments on the free rigid body and the chaotic dynamics of an underwater vehicle reveal that these reduced variational integrators possess structure-preserving properties that methods designed to preserve momentum (using the coadjoint action of the Lie group) and energy (for example, by projection) lack.

In addition we discuss how the HP integrators extend to a wider class of mechanical systems with, e.g., configuration dependent potentials and non trivial shape-space dynamics.

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Chapter 1

Introduction

1.1 Overview

This thesis is concerned with the development of efficient, structure-preserving time integrators for mechanical systems whose configuration space is a finite-dimensional Lie group. The objective will be to develop integrators that are (1) computationally efficient, (2) easy to implement, (3) structure-preserving, and (4) extensible. The first two criteria are self-explanatory. An integrator is called structure-preserving if the discrete system exactly (or to within machine precision) shares some property or properties of the continuous system. We are particularly interested in the properties that will yield an integrator that is stable for long-time simulations and that captures the correct *statistical* properties of the continuous system. We call an integrator extensible if it can be readily extended to higher-order accuracy and to a wider range of mechanical systems, for example, mechanical systems with constraints or at constant temperature. Our strategy is to revisit the ideal context of an Euler-Poincaré mechanical system from the viewpoint of Hamilton-Pontryagin mechanics.

An Euler-Poincaré (EP) system is a mechanical system whose configuration manifold is a Lie group, G, and whose Lagrangian $L : TG \to \mathbb{R}$ is fully left or right invariant under the action of that group. To be specific, this paper assumes that the Lagrangian is left-invariant. Let the tangent and cotangent bundles of G be denoted by TG and T^*G respectively, and its Lie algebra and dual be denoted by $\mathfrak{g}$ and $\mathfrak{g}^*$ respectively. The quotient space TG/G is called the *reduced space* and by the left trivialization of TG is diffeomorphic to $\mathfrak{g} = T_eG$. The restriction of the Lagrangian to the reduced space is called the reduced Lagrangian $\ell : \mathfrak{g} \to \mathbb{R}$.

Given an initial condition $(g_0, \dot{g}_0) \in TG$, the Euler-Lagrange equations for L on TG describe an initial value problem (IVP). This IVP can be left-trivialized to $G \times \mathfrak{g}$ to give

$$\dot{g} = g\xi, \quad g(a) = g_0, \tag{1.1.1}$$

$$\frac{d}{dt}\ell'(\xi) = \mathrm{ad}^*_\xi \, \ell'(\xi), \quad \xi(a) = g_0^{-1}\dot{g}_0. \tag{1.1.2}$$

Equations (1.1.1) (1.1.2) define an IVP in the *body angular velocity* $\xi(t) \in \mathfrak{g}$ and the configuration $g(t) \in G$ over the time interval $[a, b]$. However, due to the invariance of the Lagrangian with respect to the action of the Lie group, (1.1.2) is decoupled from (1.1.1). (1.1.2) is the *EP equation* and describes the dynamics reduced to $\mathfrak{g}$. To recover the configuration dynamics on G, one solves the EP equation to obtain a curve $\xi(t)$ for $t \in [a, b]$, substitutes that solution into (1.1.1), and then solves the IVP for $g(t)$ over the interval $[a, b]$, in a procedure called *reconstruction*. Consequently, (1.1.1) is called the *reconstruction equation*. A key point here is that the EP equation can be solved independently of the reconstruction equation and on a lower dimensional linear space, and often yields insight into the dynamics of the mechanical system.

The context of reduction can help design efficient, structure-preserving integrators that analogously consist of a reconstruction rule and discrete EP equations that can be solved independently of the reconstruction equation and on a lower-dimensional linear space. Specifically, the thesis presents discrete schemes that approximate the solutions of (1.1.1) (1.1.2) such that the approximation to the configuration remains on the Lie group and the approximate flow map is symplectic. The key idea is to realize the discrete schemes from a reduced variational principle. To accomplish this task, a reduced Hamilton-Pontryagin (HP) description of continuous and discrete mechanics is introduced. This description of mechanics is important in the design of variational integrators on Lie groups.

To understand its utility, the difference between reduced HP and traditional reduced variational principles is clarified. As is well known by now, there is a variational principle on $\mathfrak{g}$ known as the EP principle from which (1.1.2) follows. It is obtained by reducing Hamilton's principle for L on G using the left-trivialization of TG. There is also a variational principle on $\mathfrak{g}^*$ known as the Lie-Poisson (LP) principle [9]. Common to both of these principles is the requirement that the variations are not arbitrary as in Hamilton's principle, but are restricted to those induced by the variations of curves on the group.

The reduced HP principle skirts this issue of restricting variations by adding a Lagrange multiplier (the body angular momentum) which enforces the reconstruction equation (1.1.1) as a constraint within the principle that couples $\xi(t) \in \mathfrak{g}$ to $g(t) \in G$. As a result the continuous principle becomes more transparent, and hence, one can see a wider range of discretizations.

To be precise the reduced HP principle is not a variational principle on the reduced space $\mathfrak{g}$ or on the left-trivialized space $G \times \mathfrak{g}$. Rather this principle lies on the left trivialization of the direct sum of tangent and phase space $TG \oplus T^*G$ given by $G \times \mathfrak{g} \times \mathfrak{g}^*$. Nevertheless, the EP equations directly follow from this principle, and hence, the modifier *reduced*. The principle states that the path the continuous system follows is one that extremizes a reduced action integral.

The discrete version of this principle states that the discrete path the discrete system takes is one that extremizes a reduced action sum subject to a discrete approximation to the kinematic constraint (1.1.1). Using this discrete principle, the thesis derives and analyzes a new, extensible class of HP variational integrators (HPVI). We prove that HPVIs preserve a discrete symplectic form and a discrete momentum map. Numerical results are also provided to confirm these properties of HPVIs. Moreover, comparisons to other state-of-the-art integrators, which we refer to as FLV, KR, SW, and SW⊥ (see index of acronyms: 1.3), show that such variational integrators can be designed to be computationally efficient too. For further information about these integrators the reader is referred to [6].

Among these integrators is the semi-explicit, multi-step scheme, which we refer to as the fast Lie-Verlet method (FLV) which is the top-performing integrator in the tests. As such FLV does not directly fit within the context of this thesis namely single-step, multi-stage variational methods. However, the excellent computational performance of this method provides motivation for the development of multi-step variational integrators.

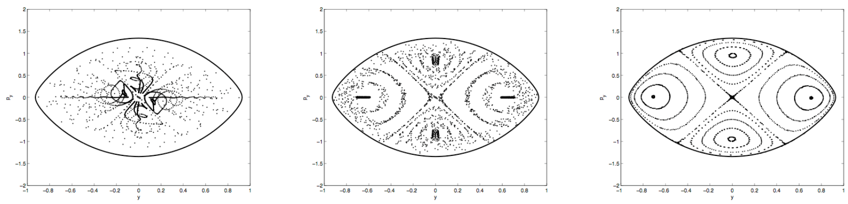
1.2 Variational Integrators

In the next paragraphs some background material is provided for the reader's convenience as well as to put the thesis into context.

Symplectic integration methods. The dynamics of seemingly unrelated conservative systems in mechanics, physics, biology, and chemistry fit the Hamiltonian formalism. Included among these are particle, rigid body, ideal fluid, solid, and plasma dynamics. The Hamiltonian flow or solution to a Hamiltonian system preserves the Hamiltonian and the symplectic form (see, for example, [36; 2]). A key consequence of symplecticity is that the Hamiltonian flow is phase-space volume preserving (Liouville's theorem). Since analytic expressions for the Hamiltonian flow are rarely available, approximations based on discretizations of time are used.

A numerical integration method which approximates a Hamiltonian flow is called symplectic if it discretely preserves a symplectic 2-form to within numerical round off [11; 44; 14] and standard otherwise. By ignoring the Hamiltonian structure, a standard method often introduces spurious dynamics, e.g., artificially corrupts phase space structures as illustrated in a computation of a Poincaré section in figure 1.2.1 using implicit Euler and a symplectic method (variational Euler).

In systems that are nonintegrable, symplectic integrators often perform much better at capturing the "right" physics compared with, for example, projection methods as illustrated in a long-time simulation of the 6-body outer solar system example in figure 1.2.2. The outer solar system example also suggests that the

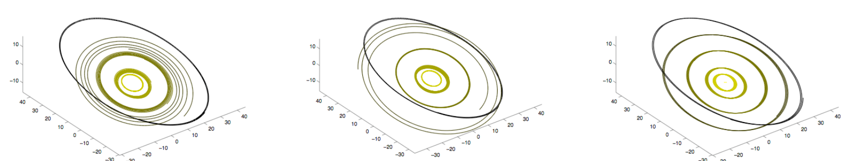


(a) Implicit Euler h=0.01 (b) Implicit Euler h=0.001 (c) Variational Euler h=0.01

Figure 1.2.1: **Spherical pendulum with $\mathbf{D_4}$ symmetric perturbation.** This figure shows a computation of a Poincaré section using implicit and a symplectic method (variational Euler). Despite the order of magnitude difference in timestep size h, implicit Euler still exhibits a systematic drift in the invariant tori, whereas variational Euler preserves them. For analysis of this mechanical system and some discussion of the numerics see [10].

structure-preserving properties of symplectic integrators are important even for large systems.

Another example being a simulation of water molecules which showed that a symplectic rigid-body integrator performed increasingly better than standard methods as the number of water molecules simulated increases [12, see figure 15].



(a) Energy Euler (b) Energy & Momentum Euler (c) Variational Euler

Figure 1.2.2: **Outer solar system.** Approximate planetary trajectories starting from the year 1994 until about the year 2500 with a timestep size of $h = 10$(days) using (from left) explicit Euler with projection onto energy (energy Euler), explicit Euler with simultaneous projection onto momentum and energy (energy and momentum Euler), and variational Euler. The orbit furthest away from the sun is Pluto in black. The planetary orbits closer to the sun are brighter. Variational Euler captures the "right" physics as compared to the benchmark while energy and energy & momentum Euler do not. For initial conditions used and more details see [15, pp. 110-113].

Design of symplectic integrators. Symplectic integrators can be derived by a variety of ways including Hamilton-Jacobi theory, symplectic splitting, and variational integration techniques.

Early investigators, guided by Hamilton-Jacobi theory, constructed symplectic integrators from generating functions which approximately solve the Hamilton-Jacobi equation [11; 44; 14]. The symplectic splitting technique is based on the property that symplectic integrators form a group, and thus, the composition of symplectic-preserving maps is also symplectic. The idea is to split the Hamiltonian into terms whose flow can be explicitly solved and then compose these individual flows in such a fashion that the composite flow is consistent and convergent with the Hamiltonian flow being simulated [25, pp. 76-80].

As we review below, variational integration techniques determine integrators from a discrete Lagrangian and associated discrete variational principle. The discrete Lagrangian can be designed to inherit the symmetry associated with the action of a Lie group, and hence by a discrete Noether's theorem, these methods can also preserve momentum invariants.

Variational integrators. Variational integration theory derives integrators for mechanical systems from discrete variational principles [47; 34; 48; 38]. The theory includes discrete analogs of the Lagrangian, Noether's theorem, the Euler-Lagrange equations, and the Legendre transform. Variational integrators can readily incorporate holonomic constraints (via Lagrange multipliers) and non-conservative effects (via their virtual work) [48; 38]. The algorithms derived from this discrete principle have been successfully tested in infinite and finite-dimensional conservative, dissipative, smooth and non-smooth mechanical systems (see [29] and references therein). Altogether, this discrete approach to mechanics stands as a self-contained theory of mechanics akin to Hamiltonian, Lagrangian or Newtonian mechanics.

Variational integrators are not distinguished by their accuracy in approximating individual trajectories, but rather in their ability to discretely preserve essential structure of the continuous system and in computing statistical properties of larger groups of orbits, such as in computing Poincaré sections or the temperature of a system. In addition to correctly computing chaotic invariant sets, evidence is mounting that variational integrators correctly compute other statistical quantities in long-time simulations. For example, in a simulation of interacting particles, Lew et al. found that variational integrators correctly compute the "temperature" (time average of the energy) over long-time intervals, whereas standard methods (even higher-order accurate ones) exhibits a systematic drift in this statistical quantity [29; 30].

Moreover, other symplectic algorithms like Newmark and Verlet can be derived within this framework by different choices of the discrete Lagrangian. In this sense it is a simple organizing principle that unifies these apparently different discretization approaches.

1.3 Structure-Preserving Lie Group Integrators

For a mechanical system on a Lie group that possesses the symmetry of that Lie group, in addition to the symplectic structure, the resulting flow preserves a momentum map associated with the Lie group symmetry. In this context there are several different strategies available to derive structure-preserving Lie group integrators; some of these are discussed here.

One strategy involves the LN method due to [45; 46]. These methods were motivated by the need to develop conserving algorithms that efficiently simulate the structural dynamics of rods and shells. For example, the configuration space of a discrete, three-dimensional finite-strain rod model, would involve N copies of $\mathbb{R}^3 \times \mathrm{SO}(3)$ where N is the number of points in the discretization of the line of centroids of the rod. For each point on the line of centroids, the orientation of the rod at that point is specified by an element of SO(3). In such models the mathematical description of the rotational degrees of freedom at these points is equivalent to the EP description of a free rigid body with added nonconservative effects due to the elastic coupling between points.

It was not apparent to these investigators that the proposed LN methods had the necessary structure-preserving properties. In fact, Simo & Wong proposed another set of algorithms which preserve momentum by using the coadjoint action on SO(3) to advance the flow [46]. Such integrators will be referred to as *coadjoint-preserving methods*. Only later did investigators understand that the midpoint rule member of the LN family with a Cayley reconstruction procedure was, in fact, a coadjoint-preserving method for SO(3) [3]. Austin et al. also numerically demonstrated the method's good performance crediting it to third-order accuracy in the discrete approximation to the Lie-Poisson structure.

Coadjoint and energy preserving methods of the Simo & Wong type that further preserve the symplectic structure were developed for SO(3) by [31; 32]. Lewis & Simo did this by defining a one-parameter family of coadjoint and energy-preserving algorithms of the Simo & Wong type in which the free parameter is a functional. The function was specified so that the resulting map defined a transformation which preserves the continuous symplectic form.

Endowing coadjoint methods with energy-preserving properties was also the subject of the works [13; 23]. Specifically, Engø & Faltinsen introduced integrators of the Runge-Kutta Munthe-Kaas type that preserved coadjoint orbits and energy using the coadjoint action on SO(3) and a numerical estimate of the gradient of the Hamiltonian. A related, novel strategy to endow coadjoint-preserving methods of Simo & Wong type with energy-preserving properties by using a simple discrete gradient was developed by [23].

Variational integration techniques have been used to derive structure-preserving integrators on Lie groups [39; 48; 35; 4; 5]. Moser and Veselov derived a variational integrator for the free rigid body by embedding SO(3) in the linear space of 3×3 matrices, $\mathbb{R}^9$, and using Lagrange multipliers to constrain the matrices to SO(3). This procedure was subsequently generalized to Lagrangian systems on more general configuration manifolds by the introduction of a discrete Hamilton's principle on the larger linear space with holonomic constraints to constrain to the configuration manifold. Wendlandt and Marsden also considered the specific example of deriving a variational integrator for the free rigid body on the Lie group S^3 by embedding S^3 into $\mathbb{R}^4$ and using a holonomic constraint [48]. The constraint ensured that the configuration update remained on the space of unit quaternions (a Lie group) and was enforced using a Lagrange multiplier.

Another approach is to use *reduction* to derive variational integrators on *reduced spaces*. Marsden, Pekarsky and Shkoller developed a discrete analog of EP reduction theory from which one could design *reduced* numerical algorithms. They did this by constructing a discrete Lagrangian on $G \times G$ that inherited the G-symmetry of the continuous Lagrangian, and restricting it to the reduced space $(G \times G)/G \sim G$. Using this discrete reduced Lagrangian and a discrete EP (DEP) principle, they derived DEP algorithms on the discrete reduced space. They also considered using generalized coordinates to parametrize this discrete reduced space, specifically the exponential map from the Lie algebra to the Lie group [35]. These techniques were applied to bodies with attitude-dependent potentials, discrete optimal control of rigid bodies, and to higher-order accuracy in [27; 28; 26].

Bobenko and Suris considered a more general case where the symmetry group is a subgroup of the Lie group G in the context of semidirect Euler-Poincaré theory [17]. They did this by writing down the discrete Euler Lagrange equations for this system and left-trivializing them [4]. For the case when the symmetry group is G itself, one recovers the DEP algorithm as pointed out in [35]. In addition, Bobenko and Suris used this theory to determine and analyze an elegant, integrable discretization of the Lagrange top [5].

The perspective in this thesis on Lie group variational integrators is different. Recognizing that Euler's equations for a rigid body are, in fact, decoupled from the dynamics on the Lie group, and more generally, that the EP equation is decoupled from the dynamics on the Lie group, the thesis aims to develop discrete variational schemes that analogously consist of a reconstruction rule and discrete EP equations that can be solved independently of the reconstruction equation and on a lower-dimensional linear space. As mentioned in the overview the central idea is to discretize the reduced HP principle in two steps. First we discretize the reconstruction equation using a Runge-Kutta-Munthe-Kaas method; and then form an HP action sum using a weighted sum of the reduced Lagrangian using the internal stages and weights of the RKMK method. The variational Euler integrators are the simplest versions of such integrators and the focus of the main body of the thesis. For higher-order accuracy or the general case of a mechanical system whose configuration space is a Lie group, the reader is referred to the future directions chapter.

Index of Acronyms

CAY: Cayley-based HPVI (§4.6)

DEP: discrete Euler-Poincaré (§1.3)

EP: Euler-Poincaré (§1.1)

EXP: Exponential-based HPVI (§4.6)

FLV: fast Lie-Verlet (§1.1)

HP: Hamilton-Pontryagin (§1.1)

HPVI: HP variational integrator (§1.1)

KR: Krysl's energy and coadjoint-preserving method (§5.6)

LP: Lie-Poisson (§1.1)

NEW: TLN-like HPVI (§5.5)

RK4: standard fourth-order accurate Runge-Kutta scheme (§6.6)

RKMK: Runge-Kutta-Munthe-Kaas scheme (§4.2.1)

SKEW: SKEW-based HPVI (§5.5)

SW: Simo & Wong explicit coadjoint-preserving method (§5.6)

SW⊥: Simo & Wong energy and coadjoint-preserving method (§5.6)

TLN: Trapezoidal Lie-Newmark method (§5.5)

VPRK: Trapezoidal Lie-Newmark method (§2.5)

1.4 Significance

There is a demand for integrators that can efficiently simulate the orientation dynamics in complex, long-duration processes such as flexible beam motion in aircraft blades, robotic arms, molecular systems, and earth-orbiting satellites; optimal control of autonomous individual and fleets of vehicles in deep-space and deep-sea missions; satellite reorientation; and the motion of articulated rigid bodies in fluids. By supplying a fast, semiexplicit structure-preserving integrator on the Lie algebra (a linear space) to simulate the dynamics on the Lie group (typically a nonlinear space), this paper addresses this need. The variational integration methods presented in this paper are also versatile. In particular, these methods are not confined to conservative systems. For example, to add nonconservative effects instead of discretizing the HP or reduced HP principle, the Lagrange-d'Alembert-Pontryagin or reduced Lagrange-d'Alembert-Pontryagin principle is discretized.

Chapter 2

HP Integrators on Vector Spaces

This chapter reviews some standard material on the HP principle in the simple context of mechanical systems whose configuration space is a real vector space equipped with the canonical symplectic form. The content comes largely from extending the standard theory on Hamiltonian systems to the HP setting [36].

2.1 HP Mechanics

Consider a mechanical system whose configuration space is a real vector space Q. Let its tangent and cotangent bundles be denoted by TQ and T^*Q respectively. Let its Lagrangian be denoted by $L : TQ \to \mathbb{R}$. Roughly speaking, Hamilton's principle states that the curve a mechanical system takes between two points on Q is an extremal of the action integral:

$$\delta \int_a^b L(q(t), \dot{q}(t))dt = 0.$$

By the variational principle of Hamilton this principle is equivalent to the curve satisfying the Euler-Lagrange equations.

Clearly, Hamilton's principle is equivalent to extremizing

$$\delta \int_a^b L(q(t), v(t))dt = 0$$

subject to the kinematic constraint $\dot{q} = v$. Introducing the Lagrange multiplier $p(t) \in T^*Q$ to enforce the constraint leads to the ***Hamilton-Pontryagin principle***

$$\delta \int_a^b [L(q(t), v(t)) + \langle p(t), \dot{q}(t) - v(t)\rangle]\, dt = 0. \tag{2.1.1}$$

This kinematic constraint may seem frivolous. However, as will be shown shortly, this principle is quite sophisticated since it builds in the Euler-Lagrange equation, the Legendre transform, and the kinematic constraint. To make these ideas precise we begin by introducing the HP action integral.

Definition 2.1.1. *The **Pontryagin bundle** is defined as the Whitney sum $TQ \oplus T^*Q$. Fix two points q_1 and q_2 on Q and an interval $[a, b]$, and define the **HP path space** as:*

$$\begin{aligned}&\mathcal{C}(q_1, q_2, [a, b])\\ &\quad = \{(q, v, p) : [a, b] \to TQ \oplus T^*Q \mid z = (g, v, p) \in C^2([a, b]), q(a) = q_1, q(b) = q_2\},\end{aligned}$$

*and the **HP action integral** $\mathfrak{G} : \mathcal{C}(q_1, q_2, [a, b]) \to \mathbb{R}$ by:*

$$\mathfrak{G}(z) = \int_a^b [L(q(t), v(t)) + \langle p(t), \dot{q}(t) - v(t)\rangle]\, dt.$$

The Pontryagin bundle is a vector bundle over Q whose fiber at $q \in Q$ is the vector space $T_qQ \oplus T_q^*Q$. The HP path space is a smooth infinite-dimensional manifold. It can be shown that its tangent space at $(q, v, p) \in \mathcal{C}(q_1, q_2, [a, b])$ consists of $C^2([a, b])$ maps $w = (q, v, p, \delta q, \delta v, \delta p) : [a, b] \to T(TQ \oplus T^*Q)$ such that $\delta q(a) = \delta q(b) = 0$. The following theorem was introduced and proved in [52]. It should be emphasized that the Lagrangian could be degenerate in the theorem, i.e., its Hessian matrix with respect to v may not be invertible.

Theorem 2.1.2 (Variational Principle of Hamilton-Pontryagin)**.** *Let L be a Lagrangian on TQ with continuous partial derivatives of second order with respect to q and v. A curve $c = (q, v, p) : [a, b] \to TQ \oplus T^*Q$ joining $q_1 = q_0(a)$ to $q_2 = q_0(b)$*

satisfies the HP equations:

$$\dot{q} = v, \tag{2.1.2}$$

$$\dot{p} = \frac{\partial L}{\partial q}(q, v), \tag{2.1.3}$$

$$p = \frac{\partial L}{\partial v}(q, v), \tag{2.1.4}$$

if c is a critical point of the function $\mathfrak{G} : \mathcal{C}(q_1, q_2, [a, b]) \to \mathbb{R}$, that is, $\mathbf{d}\mathfrak{G}(c) = 0$.

Proof. The differential of the HP action integral is given by,

$$\mathbf{d}\mathfrak{G}(c) \cdot (\delta q, \delta v, \delta p) = \int_a^b \left[\frac{\partial L}{\partial q}(q, v) \cdot \delta q + \frac{\partial L}{\partial v}(q, v) \cdot \delta v + \langle \delta p, \dot{q} - v \rangle + \langle p, \delta \dot{q} - \delta v \rangle \right] dt.$$

Integrating by parts, using the endpoint conditions (i.e., $\delta q(a) = \delta q(b) = 0$), and simplifying yields,

$$\mathbf{d}\mathfrak{G}(c) \cdot (\delta q, \delta v, \delta p) = \int_a^b \left[\left(\frac{\partial L}{\partial q}(q, v) - \dot{p} \right) \cdot \delta q + \delta p \cdot (\dot{q} - v) + \left(\frac{\partial L}{\partial v}(q, v) - p \right) \cdot \delta v \right] dt.$$

If c is a critical point of $\mathfrak{G}$ then $\mathbf{d}\mathfrak{G}(c) \cdot w = 0$ for all $w \in T_c\mathcal{C}(z_1, z_2, [a, b])$, and hence, the equations follow from a basic lemma from variational calculus. ■

For the purpose of this thesis, we restrict our subsequent discussion to non-degenerate Lagrangians. However, the reader is referred to the following papers as a starting point to generalize the HP integrators in this thesis to degenerate Lagrangian systems: [51; 52].

2.2 HP Equations and the Fiber Derivative

By introducing the kinematic constraint, we were able to derive an action integral on $\mathcal{C}(z_1, z_2, [a, b])$ whose extremal is a solution to the HP equations. Eliminating v

using (2.1.4) yields an initial value problem on T^*Q. Thus, the resulting extremal can be thought of as an integral curve of a vector field on T^*Q. It is instructive to compare this procedure of deriving a vector field on T^*Q to the usual way one passes from the second-order, Euler-Lagrange equations on TQ to Hamilton's equations on T^*Q.

Recall that starting with an L on TQ we pass to T^*Q via the Legendre transform of L to obtain the Hamiltonian $H : T^*Q \to \mathbb{R}$:

$$H(q,p) = \langle p, v(q,p)\rangle - L(q, v(q,p)); \quad \frac{\partial L}{\partial v}(q, v(q,p)) = p.$$

Non-degeneracy of L and the implicit function theorem ensure that one can solve for v as a function of (q,p). The latter equation is known as the fiber derivative of L. Hamilton's equations then follow from Hamilton's phase space principle,

$$\dot{q} = \frac{\partial H}{\partial p}(q,p), \tag{2.2.1}$$

$$\dot{p} = -\frac{\partial H}{\partial q}(q,p). \tag{2.2.2}$$

However, these equations are not yet in the form of the HP equations. To put (2.2.2) in the desired form, one has to differentiate the Legendre transform of L with respect to v. Likewise to put (2.2.1) in the correct form, one performs a Legendre transform of H with respect to p to obtain:

$$L(q, v(q,p)) = \langle p, v(q,p)\rangle - H(q,p); \quad \frac{\partial H}{\partial p}(q,p) = v(q,p).$$

The kinematic constraint then follows from the fiber derivative of H. In summary, to obtain the HP equations (a vector field on T^*Q) from a Lagrangian L on TQ one has to perform a double Legendre transform or, if you prefer, two fiber derivatives. On the other hand, to derive the HP equations from the HP principle the Legendre transform did not need to be introduced. Instead the Legendre transform follows directly from the principle.

2.3 Symplecticity of HP Flow

Consider the symplectic vector space (T^*Q, Ω) where Ω is the canonical symplectic form and Q is n-dimensional. The matrix of Ω is the canonical one

$$\mathbb{J} := \begin{bmatrix} \mathbf{0} & \mathbf{I} \\ -\mathbf{I} & \mathbf{0} \end{bmatrix},$$

where $\mathbf{0}$ is the $n \times n$ zero matrix and $\mathbf{I}$ is the $n \times n$ identity matrix. Strictly speaking the HP equations define a differential-algebraic system of equations on $TQ \oplus T^*Q$. However, one can eliminate v using (2.1.4) to obtain an IVP on T^*Q. That is, given an initial condition $(q(a), p(a)) \in T^*Q$ and a time interval $[a, b]$ one can integrate (2.1.2) – (2.1.4) to obtain a map $F_{HP} : T^*Q \to T^*Q$. We will prove here that this map is symplectic, i.e., it preserves the canonical symplectic form. Define the following vector field $X_{HP} : T^*Q \to T(T^*Q)$

$$X_{HP}(q, p) = \left(v(q, p), \frac{\partial L}{\partial q}(q, v(q, p)) \right),$$

where $v(q, p)$ is determined by (2.1.4). Let us assume it is smooth. We will show that this vector field is Hamiltonian if L is non-degenerate. Computing the Jacobian matrix of the map using (2.1.4) gives,

$$DX_{HP}(q, p) = \begin{bmatrix} v_q & v_p \\ L_{qq} + L_{qv}v_q & L_{vq}v_p \end{bmatrix} = \begin{bmatrix} -L_{vv}^{-1}L_{vq} & L_{vv}^{-1} \\ L_{qq} - L_{qv}L_{vv}^{-1}L_{qv} & L_{vq}L_{vv}^{-1} \end{bmatrix}.$$

Observe that DX_{HP} is Ω-skew since

$$\mathbb{J}DX_{HP} = \begin{bmatrix} L_{qq} - L_{qv}L_{vv}^{-1}L_{qv} & L_{vq}L_{vv}^{-1} \\ L_{vv}^{-1}L_{vq} & -L_{vv}^{-1} \end{bmatrix}$$

is symmetric. Hence, X_{HP} is Hamiltonian and its flow is symplectic.

Theorem 2.3.1. *The flow of X_{HP} preserves the canonical symplectic form, i.e., $F_{HP}^*\Omega = \Omega$.*

2.4 Discretization of Kinematic Constraint

Speaking informally, to obtain a discrete HP description of a mechanical system, the HP action integral is approximated by a sum whose extremal is assumed to be the discrete path the mechanical system takes. This procedure was implemented from the viewpoint of discrete Lagrangians in [22]. That paper also considers an interesting application of a discrete HP time integrator to a problem in nonlinear elasticity—an animation of a rabbit hopping. However, the paper does not specify how to design the discrete Lagrangian to, e.g., achieve higher-order accuracy. Here we introduce a specific discretization of the HP principle which will give a family of integrators that include higher-order accurate members.

To discretize the HP action integral one needs to replace the continuous Lagrangian and kinematic contraint by discrete approximants. We begin by setting up and motivating the time discretization of the kinematic constraint (cf. (2.1.2)). Let $[a, b]$ and N be given and define the fixed step size $h = (b - a)/(N - 1)$ and $t_k = hk$. In what follows we regard $(q(t), v(t)) \in TQ$.

A discretization of the kinematic constraint can be obtained by introducing a discrete sequence $\{q_k\}_{k=0}^{N}$ such that $q_k \in Q$ and a map $\varphi : Q \times Q \to TQ$ defined as:

$$\varphi(q_k, q_{k+1}) = (\kappa(q_k, q_{k+1}), \Gamma(q_k, q_{k+1})), \quad \Gamma(q_k, q_{k+1}) \in T_{\kappa(q_k, q_{k+1})}Q.$$

The discrete kinematic constraint can then be written in abstract form as

$$\varphi(q_k, q_{k+1}) = (\kappa(q_k, q_{k+1}), v(t_k)) \in TQ, \quad \Gamma(q_k, q_{k+1}) \in T_{\kappa(q_k, q_{k+1})}Q.$$

That is, the maps φ and κ are not specified. For example, since Q is a vector space one can define the following forward difference approximation:

$$\varphi(q_k, q_{k+1}) = \left(q_k, \frac{q_{k+1} - q_k}{h} \right)$$

in terms of which the kinematic constraint becomes

$$\frac{q_{k+1} - q_k}{h} = v(t_k).$$

As opposed to taking this abstract route, we will specify these maps by using a Runge-Kutta discretization of the kinematic constraint since the theory on Runge-Kutta methods (order conditions, stability, and implementation) is mature. See, for instance, [16].

Definition 2.4.1. *Consider the first order differential equation*

$$\dot{q} = f(t, q), \quad q(0) = q_0, \quad q(t) \in Q. \tag{2.4.1}$$

Let $b_i, a_{ij} \in \mathbb{R}$ $(i, j = 1, \cdots, s)$ *and let* $c_i = \sum_{j=1}^{s} a_{ij}$. *An* ***s-stage Runge-Kutta*** *approximation is given by*

$$Q_k^i = q_k + h \sum_{j=1}^{s} a_{ij} f(t_k + c_j h, Q_k^j), \quad i = 1, \cdots, s, \tag{2.4.2}$$

$$q_{k+1} = q_k + h \sum_{j=1}^{s} b_j f(t_k + c_j h, Q_k^j). \tag{2.4.3}$$

If $a_{ij} = 0$ *for* $i \leq j$ *the Runge-Kutta method is called explicit, and implicit otherwise. The vectors* q_k *and* Q_k^i *are called external and internal stage vectors, respectively.*

It follows that an s-stage Runge-Kutta method is fully determined by its $s \times s$ matrix and s-vector: a and b. These coefficients in tabular form:

$$\begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array}$$

are sometimes called the Butcher tableau in honor of J. C. Butcher's research on multistage Runge-Kutta methods. The implicit function theorem ensures that for

h sufficiently small one can solve (2.4.2)-(2.4.3) for the $s+1$ unknown vectors given q_k. It should be mentioned that collocation methods are an instance of s-stage Runge-Kutta methods.

Definition 2.4.2. *Let $q(t)$ be the exact solution of (2.4.1). An s-stage Runge-Kutta method is of* ***order p*** *if for sufficiently smooth functions f the following local error condition holds:*

$$\|q(h) - q_1\| \leq Kh^{p+1},$$

where $\|\cdot\|$ is the Euclidean norm and K is a constant.

Applying an s-stage Runge-Kutta method to the kinematic constraint $\dot{q} = v(t)$ where $(q(t), v(t)) \in TQ$ gives:

$$Q_k^i = q_k + h\sum_{j=1}^{s} a_{ij} v(t_k + c_j h), \quad i = 1, \cdots, s, \tag{2.4.4}$$

$$q_{k+1} = q_k + h\sum_{j=1}^{s} b_j v(t_k + c_j h). \tag{2.4.5}$$

Fig. 2.4.1 illustrates how the internal and external stage vectors are related. In particular, it shows that the velocities $V_k^j = v(t_k + c_j h)$ are regarded as tangent vectors at Q_k^j. Since Q is a vector space the precise location of these tangent vectors is not essential. However, it will be helpful to be systematic about their location since we will, in subsequent chapters, extend these ideas to Lie groups. We will find that this discretization of the kinematic constraint will provide a rich class of variational integrators.

2.5 VPRK Integrator on Vector Spaces

The variational partitioned Runge-Kutta (VPRK) method will be derived from a discretization of the HP action integral in which the kinematic constraint is replaced with its discrete approximant: (2.4.4) (2.4.5). As in the continuous theory, the Lagrange multiplier in the external stages corresponds to the linear momentum.

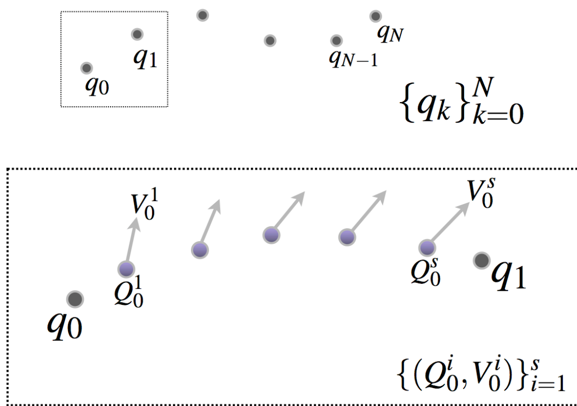


Figure 2.4.1: **Discretization of kinematic constraint.** The external and internal stage updates of the Runge-Kutta discretization of the kinematic constraint are shown. The vectors V_k^j, $j = 1, \cdots, s$ are regarded as being based at Q_k^j, i.e., $V_k^j \in T_{Q_k^j} Q$.

Definition 2.5.1. *Fix two points q_1 and q_2 on Q and define the* ***discrete VPRK path space*** *as:*

$$\mathcal{C}_d = \{(q, p, \{Q^i, V^i, P^i\}_{i=1}^s)_d : \{t_k\}_{k=0}^N \to T^*Q \times (TQ \oplus T^*Q)^s \mid \\ q(0) = q_1, q(t_N) = q_2\},$$

and the ***discrete VPRK action sum*** $\mathfrak{G}_d : \mathcal{C}_d(q_1, q_2) \to \mathbb{R}$ *by:*

$$\mathfrak{G}_d = \sum_{k=0}^{N-1} \sum_{i=1}^{s} h \left[b_i L(Q_k^i, V_k^i) + \left\langle p_k^i, (Q_k^i - q_k)/h - \sum_{j=1}^{s} a_{ij} V_k^j \right\rangle \right. \\ \left. + \left\langle p_{k+1}, (q_{k+1} - q_k)/h - \sum_{j=1}^{s} b_j V_k^j \right\rangle \right].$$

A family of partitioned Runge-Kutta methods will be shown to be extremals of this discrete action sum; included among these are the symplectic Euler, Störmer-Verlet, Gauss collocation methods, and the Lobatto IIIA-IIIB pair. Previous investigators have shown that the discrete Hamiltonian map associated to the discrete

Lagrangian

$$L_h = h\sum_{i=1}^{s} b_i L(Q_k^i, V_k^i)$$

is a symplectic partitioned Runge-Kutta method [38]. We extend this theorem by proving that an extremal of a discrete HP action sum satisfies a symplectic partitioned Runge-Kutta method applied to the HP equations. In addition it will be shown that the coefficients of the scheme satisfy the well-known conditions for symplecticity of a partitioned Runge-Kutta method [15].

Theorem 2.5.2. *Let L be a Lagrangian on TQ with continuous partial derivatives of second order with respect to q and v. A discrete curve $c_d \in \mathcal{C}_d(q_1, q_2)$ satisfies the following partitioned Runge-Kutta method applied to (2.1.2)-(2.1.4):*

$$\begin{aligned}
Q_k^i &= q_k + h\textstyle\sum_{j=1}^s a_{ij} V_k^j, \\
q_{k+1} &= q_k + h\textstyle\sum_{j=1}^s b_j V_k^j, \\
P_k^i &= p_k + h\textstyle\sum_{j=1}^s \left(b_j - b_j \frac{a_{ji}}{b_i}\right) \frac{\partial L}{\partial q}(Q_k^j, V_k^j), \\
p_{k+1} &= p_k + h\textstyle\sum_{j=1}^s b_j \frac{\partial L}{\partial q}(Q_k^j, V_k^j), \\
P_k^i &= \frac{\partial L}{\partial v}(Q_k^i, V_k^i).
\end{aligned} \tag{2.5.1}$$

for $i = 1, \cdots, s$ and $k = 0, \cdots, N-1$, if it is a critical point of the function $\mathfrak{G}_d : \mathcal{C}_d(q_1, q_2) \to \mathbb{R}$, that is, $\mathbf{d}\mathfrak{G}_d(c_d) = 0$. Moreover, the discrete flow map defined by the above scheme is symplectic.

Proof. The differential of $\mathfrak{G}_d(c_d)$ in the direction $z = (\{\delta q_k, \delta p_k\}, \{\delta Q_k^i, \delta V_k^i, p_k^i\}_{i=1}^s)$ is given by:

$$\begin{aligned}
d\mathfrak{G}_d \cdot z = &\sum_{k=0}^{N-1}\sum_{i=1}^{s} hb_i \left[\frac{\partial L}{\partial q}(Q_k^i, V_k^i)\cdot \delta Q_k^i + \frac{\partial L}{\partial v}(Q_k^i, V_k^i)\cdot \delta V_k^i\right] \\
&+ h\left[\left\langle p_k^i, (\delta Q_k^i - \delta q_k)/h - \sum_{j=1}^s a_{ij}\delta V_k^j\right\rangle + \left\langle p_{k+1}, (\delta q_{k+1} - \delta q_k)/h - \sum_{j=1}^s b_j \delta V_k^j\right\rangle\right] \\
&+ h\left[\left\langle \delta p_k^i, (Q_k^i - q_k)/h - \sum_{j=1}^s a_{ij} V_k^j\right\rangle + \left\langle \delta p_{k+1}, (q_{k+1} - q_k)/h - \sum_{j=1}^s b_j V_k^j\right\rangle\right].
\end{aligned}$$

Collecting terms with the same variations and summation by parts using the boundary conditions $\delta q_0 = \delta q_N = 0$ gives,

$$\begin{aligned} d\mathfrak{G}_d \cdot z = \sum_{k=0}^{N-1} \sum_{i=1}^{s} \left(h b_i \frac{\partial L}{\partial q}(Q_k^i, V_k^i) + p_k^i \right) \cdot \delta Q_k^i + \left(-p_{k+1} + p_k - \sum_{i=1}^{s} p_k^i \right) \cdot \delta q_k \\ + h \left(b_i \frac{\partial L}{\partial v}(Q_k^i, V_k^i) - \sum_{j=1}^{s} \frac{a_{ji}}{b_i} p_k^j - b_i p_{k+1} \right) \cdot \delta V_k^i \\ + h \left\langle \delta p_k^i, (Q_k^i - q_k)/h - \sum_{j=1}^{s} a_{ij} V_k^j \right\rangle \\ + h \left\langle \delta p_{k+1}, (q_{k+1} - q_k)/h - \sum_{j=1}^{s} b_j V_k^j \right\rangle . \end{aligned}$$

Since $d\mathfrak{G}_d(c_d) = 0$ implies that $d\mathfrak{G}_d \cdot z = 0$ for all $z \in T_{c_d}\mathcal{C}_d$, one arrives at the desired equations with the elimination of p_k^i and the introduction of the internal stage variables $P_k^i = \partial L/\partial v(Q_k^i, V_k^i)$ for $i = 1, \cdots, s$. To see that the scheme is symplectic, one checks that the coefficients of the partitioned Runge-Kutta scheme (2.5.1) satisfy the following condition of symplecticity (see, e.g., [15])

$$b_i \bar{a}_{ij} + \bar{b}_j a_{ji} = b_i \bar{b}_j, \quad b_i = \bar{b}_i \quad \text{for } i, j = 1, \cdots, s.$$

The second condition is clearly satisfied and the first is as well since $\bar{a}_{ij} = b_j - b_j a_{ji}/b_i$. ■

2.6 Variational Euler on Vector Spaces

As examples of a VPRK integrator we consider two simples case: 1-stage, explicit and implicit Euler discretizations of the kinematic constraint defined by the following Butcher tableaus:

$$\begin{array}{c|c} 0 & \\ \hline & 1 \end{array}\ , \qquad\qquad \begin{array}{c|c} 1 & 1 \\ \hline & 1 \end{array}\ .$$

explicit Euler   implicit Euler

The corresponding VPRK action sums take the following simple forms:

$$\mathfrak{G}_d^e = \sum_{k=0}^{N-1} h \left[L(q_k, V_k^1) + \left\langle p_{k+1}, (q_{k+1} - q_k)/h - V_k^1 \right\rangle \right] \qquad \mathfrak{G}_d^i = \sum_{k=0}^{N-1} h \left[L(q_{k+1}, V_k^1) + \left\langle p_{k+1}, (q_{k+1} - q_k)/h - V_k^1 \right\rangle \right]$$

and the corresponding discrete HP equations are given by:

$$\begin{aligned} q_{k+1} &= q_k + hV_k^1(q_k, p_{k+1}), & q_{k+1} &= q_k + hV_k^1(q_{k+1}, p_k), \\ p_{k+1} &= p_k + h\frac{\partial L}{\partial q}(q_k, V_k^1(q_k, p_{k+1})), & p_{k+1} &= p_k + h\frac{\partial L}{\partial q}(q_{k+1}, V_k^1(q_{k+1}, p_k)), \\ p_{k+1} &= \frac{\partial L}{\partial v}(q_k, V_k^1(q_k, p_{k+1})), & p_k &= \frac{\partial L}{\partial v}(q_{k+1}, V_k^1(q_{k+1}, p_k)). \end{aligned}$$

We will call these methods ***variational Euler methods***. A major goal of this thesis is to generalize these methods to Lie groups using HP mechanics. In the vector space context, these methods are also called symplectic Euler methods. By eliminating V_k^1 in the above equations using the discrete fiber derivative, both sets of equations implicitly define update schemes $\varphi : T^*Q \to T^*Q$ given (q_k, p_k). Regarding T^*Q as a symplectic vector space with the canonical symplectic form Ω, one can check that the maps are symplectic directly. For example, consider the map given by the explicit Euler discretization of the kinematic constraint. Its Jacobian matrix is given by,

$$D\varphi = \begin{bmatrix} \mathbf{I} + hA & hB^{-1} \\ hL_{qq} + hL_{qv}A & \mathbf{I} + hL_{qv}B^{-1} \end{bmatrix},$$

where $B = (L_{vv} - hL_{qv})$, $A = B^{-1}(hL_{qq} - L_{qv})$ and $\mathbf{I}$ is the $n \times n$ identity matrix. It is then easy to confirm that:

$$(D\varphi)^T \mathbb{J} D(\varphi) = \mathbb{J},$$

and hence the map φ is symplectic.

In closing let us summarize what has been done so far. The chapter began with a review of HP mechanics in the continuous setting. The integrand of the

HP action integral consisted of the Lagrangian added to the kinematic constraint enforced using a Lagrange multiplier (the linear momentum). To discretize this action integral, the first step involved a discretization of the kinematic constraint using an s-stage Runge-Kutta method. The integral of the continuous Lagrangian was approximated by a weighted sum of the Lagrangian evaluated at internal stages using the weights given by the s-stage Runge-Kutta method. The main result of the chapter stated that an extremal of the resulting action sum satisfies the VPRK scheme. The chapter concluded with the simplest example of such a scheme, namely the variational Euler integrator.

Chapter 3

HP Mechanics for EP Systems

A key goal in subsequent chapters is to generalize continuous and discrete HP mechanics as presented in chapter 2 from configuration spaces that are vector spaces to Lie groups. Our strategy will be to start with an analysis of the ideal case of an EP system. The general case of a mechanical system whose configuration space is a Lie group is not much harder and will be deferred to chapter 7. As we proceed confirming symplecticity algebraically as employed in chapter 2 will become cumbersome. Instead, the so-called variational proof of symplecticity will be adopted in what follows. We will also show other interesting consequences of the variational structure of EP systems such as momentum map preservation.

3.1 Reduced HP Principle

Consider a mechanical system whose configuration space is a Lie group G. Let its tangent and cotangent bundles be denoted TG and T^*G respectively, and its Lie algebra and dual of the Lie algebra given by $\mathfrak{g}$ and $\mathfrak{g}^*$ respectively. Let its Pontryagin bundle be denoted by $TG \oplus T^*G$.

In this section the left-trivialization of the HP principle for a left-invariant Lagrangian $L : TG \to \mathbb{R}$ will be derived. Left-invariance means that the Lagrangian is invariant under the left action of G on itself and hence on TG; i.e., $L(g, \dot{g}) = L(hg, h\dot{g})$ for all $h \in G$, where the left action is denoted by simple concatentation. And in particular, taking $h = g^{-1}$, we find that $L(g, \dot{g}) = L(e, g^{-1}\dot{g})$

where $e \in G$ is the identity. This identity motivates the following definition.

Definition 3.1.1. *The* ***reduced Lagrangian*** $\ell : \mathfrak{g} \to \mathbb{R}$*, is defined as the left trivialization of the Lagrangian, i.e.,* $\ell = L(e, \xi)$ *where* $\xi = g^{-1}\dot{g} \in \mathfrak{g}$.

As reviewed in the vector-space context, the HP principle unifies the Hamiltonian and Lagrangian descriptions of a mechanical system [51; 52]. It states the following critical point condition on $TG \oplus T^*G$,

$$\delta \int_a^b \left[L(g, v) + \langle p, \dot{g} - v \rangle \right] \, dt = 0,$$

where $(g(t), v(t), p(t)) \in TG \oplus T^*G$ are varied arbitrarily and independently with endpoint conditions $g(a)$ and $g(b)$ fixed. This principle builds in the Legendre transformation as well as the Euler–Lagrange equations into one principle.

It will be shown that the HP principle for systems on Lie groups is equivalent to the reduced HP principle:

$$\delta \int_a^b \left[\ell(\xi) + \left\langle \mu, g^{-1}\dot{g} - \xi \right\rangle \right] \, dt = 0,$$

where there are no constraints on the variations; that is, the curves $\xi(t) \in \mathfrak{g}$, $\mu(t) \in \mathfrak{g}^*$ and $g(t) \in G$ can be varied arbitrarily. To see this, we proceed as follows.

Definition 3.1.2. *Fixing the interval* $[a, b]$*, define* ***path space*** *as*

$$\mathcal{C}(TG \oplus T^*G) = \{ (g, v, p) : [a, b] \to TG \oplus T^*G \mid (g, v, p) \in C^2([a, b]) \}.$$

Let $S : \mathcal{C}(TG \oplus T^*G) \to \mathbb{R}$ *denote the* ***HP action integral****,*

$$S(g, v, p) = \int_a^b \left[L(g, v) + \langle p, \dot{g} - v \rangle \right] \, dt.$$

Similarly, define the ***reduced path space*** *as*

$$\mathcal{C}(G \times \mathfrak{g} \times \mathfrak{g}^*) = \{ (g, \xi, \mu) : [a, b] \to G \times \mathfrak{g} \times \mathfrak{g}^* \mid (g, \xi, \mu) \in C^2([a, b]) \}.$$

The ***reduced HP action integral*** $s : \mathcal{C}(G \times \mathfrak{g} \times \mathfrak{g}^*) \to \mathbb{R}$ *is defined as*

$$s(g, \xi, \mu) = \int_a^b \left[\ell(\xi) + \left\langle \mu, TL_{g^{-1}}\dot{g} - \xi \right\rangle \right] \, dt.$$

Left-invariance of L gives the following relationship between S and s,

$$\begin{aligned} S(g, v, p) &= \int_a^b \left[L(L_{g^{-1}}g, TL_{g^{-1}}v) + \left\langle p, TL_g TL_{g^{-1}}(\dot{g} - v) \right\rangle \right] \, dt \\ &= \int_a^b \left[L(e, TL_{g^{-1}}v) + \left\langle TL_g^* p, TL_{g^{-1}}(\dot{g} - v) \right\rangle \right] \, dt \\ &= \int_a^b \left[\ell(\xi) + \left\langle \mu, TL_{g^{-1}}\dot{g} - \xi \right\rangle \right] \, dt \\ &= s(g, \xi, \mu) \end{aligned}$$

where $\xi = g^{-1}v \in \mathfrak{g}$ and $\mu = g^{-1}p \in \mathfrak{g}^*$. From this equality one can derive the following key theorem.

Theorem 3.1.3. *Let G be a Lie group and $L : TG \to \mathbb{R}$ be a left invariant Lagrangian. Let $\ell : \mathfrak{g} \to \mathbb{R}$ be its restriction to the identity. Then the following are equivalent*

1. *Hamilton's principle for L on G,*

$$\delta \int_a^b L(g, \dot{g}) dt = 0,$$

holds, for arbitrary variations $g(t)$ with endpoint conditions $g(a)$ and $g(b)$ fixed;

2. *the EP variational principle holds on $\mathfrak{g}$,*

$$\delta \int_a^b \ell(\xi) dt = 0,$$

using variations of the form

$$\delta\xi = \dot{\eta} + \mathrm{ad}_\xi \, \eta,$$

where $\eta(a) = \eta(b) = 0$ and $\xi = g^{-1}\dot{g}$; i.e., $\xi = TL_{g^{-1}}\dot{g}$;

3. *the HP principle,*

$$\delta \int_a^b [L(g,v) + \langle p, \dot{g} - v\rangle]\, dt = 0,$$

holds, where $(g(t), v(t), p(t)) \in TG \oplus T^*G$, can be varied arbitrarily and independently with endpoint conditions $g(a)$ and $g(b)$ fixed;

4. *the reduced HP principle,*

$$\delta \int_a^b \left[\ell(\xi) + \left\langle \mu, g^{-1}\dot{g} - \xi \right\rangle\right]\, dt = 0,$$

holds, where $(g(t), \xi(t), \mu(t)) \in G \times \mathfrak{g} \times \mathfrak{g}^*$ can be varied arbitrarily and independently with endpoint conditions $g(a)$ and $g(b)$ fixed.

Just as the HP principle unifies the Hamiltonian and Lagrangian descriptions of mechanical systems, the reduced HP principle unifies the EP and Lie-Poisson descriptions on $\mathfrak{g}$ and $\mathfrak{g}^*$ respectively [37; 9].

The free rigid body on the Lie group S^3 furnishes a simple example of various representations of variational principles on Lie groups and is discussed below. This rolling example will also clarify the differences between the variational perspective of this paper and that of [48].

3.2 Example: Free Rigid Body on $\mathbf{S^3}$

The set of unit quaternions is the three-sphere,

$$S^3 = \{(x_s, \mathbf{x}_v) : x_s \in \mathbb{R}, \mathbf{x}_v \in \mathbb{R}^3, x_s^2 + \|\mathbf{x}_v\|^2 = 1\},$$

which is a Lie group under the operation,

$$a \star b = (a_s b_s - \mathbf{a}_v \cdot \mathbf{b}_v, a_s \mathbf{b}_v + b_s \mathbf{a}_v + \mathbf{a}_v \times \mathbf{b}_v),$$

for $a = (a_s, \mathbf{a}_v), b = (b_s, \mathbf{b}_v) \in S^3$. Every unit quaternion $g = (x_s, \mathbf{x}_v)$ has a conjugate $g^* = (x_s, -\mathbf{x}_v)$ which is also its inverse, i.e., $g \star g^* = (1, \mathbf{0}) = e \in S^3$. For more information on quaternions the reader is referred to [36, §9.2].

Define the unconstrained Lagrangian of the free rigid body, $L : T\mathbb{R}^4 \to \mathbb{R}$, in terms of quaternions,[1]

$$L(g, \dot{g}) = \frac{1}{2}(2g^* \star \dot{g})^T \begin{bmatrix} 0 & 0 \\ 0 & J \end{bmatrix} (2g^* \star \dot{g})$$

where J is a diagonal matrix whose entries are the principal moments of inertia of the body [48]. Observe that this Lagrangian is left-invariant with respect to the action of S^3 since for all $B \in S^3$,

$$L(g, \dot{g}) = L(Bg, B\dot{g}).$$

Consider the restriction of L to TS^3 by a generalized coordinate formulation and let $L^c : TS^3 \to \mathbb{R}$ denote this restricted Lagrangian defined as $L^c = L|_{TS^3}$. And since the Lie algebra of S^3 is isomorphic to the pure quaternions $\mathbb{R}^3$ relative to the Lie bracket given by twice the cross product, one can write ξ as

$$\xi = g^{-1} \star \dot{g} = \frac{1}{2}(0, \mathbf{\Omega}). \tag{3.2.1}$$

The factor 1/2 is introduced to ensure that the vectorial part of the Lie algebra variable agrees with the usual definition of the body angular velocity for the free rigid body and that the Lie bracket on $\mathbb{R}^3$ is just the usual cross product. By definition, the reduced Lagrangian ℓ is obtained by restricting L^c to the reduced space TG/G,

$$\ell(\mathbf{\Omega}) = L^c(e, 1/2(0, \mathbf{\Omega})).$$

[1] Alternatively, the unconstrained Lagrangian of the free rigid body can be defined in terms of 3×3 matrices as $L : T\mathbb{R}^9 \to \mathbb{R}$. To constrain these matrices to the Lie group SO(3) one uses an orthogonality constraint. The SO(3)-perspective is adopted in chapter 5.

Define a vector-valued constraint function, $\varphi : \mathbb{R}^4 \to \mathbb{R}$, as

$$\varphi(g) = \sqrt{g^T g} - 1,$$

such that $\varphi^{-1}(0)$ is the submanifold S^3 of $\mathbb{R}^4$. Then theorem 3.1.3 specialized to this mechanical system states that the following are equivalent,

1. Hamilton's principle for L
   - restricted to S^3 using generalized coordinates L^c,

     $$\delta \int_a^b L^c(g, \dot{g}) dt = 0$$

     holds, for arbitrary variations $g(t) \in S^3$
   - on $\mathbb{R}^4$ using constrained coordinates,

     $$\delta \int_a^b \left[L(g, \dot{g}) + \lambda \varphi(g) \right] dt = 0$$

     holds, for arbitrary variations $g(t) \in \mathbb{R}^4$

   with $g(a)$ and $g(b)$ fixed;
2. the EP variational principle holds on $\mathbb{R}^3$,

   $$\delta \int_a^b \ell(\mathbf{\Omega}) dt = 0$$

   using variations of the form

   $$\delta \mathbf{\Omega} = \dot{\Sigma} + \mathbf{\Omega} \times \Sigma$$

   where $\Sigma(a) = \Sigma(b) = 0$ and $\mathbf{\Omega}$ satisifes (3.2.1);
3. the HP principle

- using generalized coordinates,

$$\delta \int_a^b \left[L^c(g, v) + \langle p, \dot{g} - v \rangle \right] \, dt = 0,$$

  holds, where $(g(t), v(t), p(t)) \in TS^3 \oplus T^*S^3$, can be varied arbitrarily and independently

- using constrained coordinates,

$$\delta \int_a^b \left[L(g, v) + \langle p, \dot{g} - v \rangle + \lambda \varphi(g) \right] \, dt = 0,$$

  holds, where $(g(t), v(t), p(t)) \in T\mathbb{R}^4 \oplus T^*\mathbb{R}^4$, can be varied arbitrarily and independently

with $g(a)$ and $g(b)$ fixed;

4. the reduced HP principle

$$\delta \int_a^b \left[\ell(\mathbf{\Omega}) + \left\langle (0, \mathbf{\Pi}), g^{-1} \star \dot{g} - \frac{1}{2}(0, \mathbf{\Omega}) \right\rangle \right] \, dt = 0,$$

   holds, where $(g(t), \mathbf{\Omega}(t), \mathbf{\Pi}(t)) \in S^3 \times \mathbb{R}^3 \times \mathbb{R}^3$ can be varied arbitrarily and independently with endpoint conditions $g(a)$ and $g(b)$ fixed.

The example illustrates that Hamilton's and the HP principle in terms of generalized coordinates are equivalent to Hamilton's and the HP principle using constrained coordinates and the Lagrange multiplier method to enforce the constraint respectively. Moreover, it concretely shows the reduced HP and EP variational principles for this choice of Lie group.

3.3 Unreduced HP Flow

The equations of motion can be obtained from the HP principle as follows. The variations of the HP action integral with respect to p and v give

$$\delta p \implies v = \dot{g}, \quad \text{(kinematic constraint)}, \tag{3.3.1}$$

$$\delta v \implies p = D_2 L(g, v), \quad \text{(Legendre transform)}. \tag{3.3.2}$$

Note that (3.3.1) is a constraint equation relating $\dot{g}$ to v with associated Lagrange multiplier given by the momentum p; see, e.g., [22]. We assume throughout this paper that the Legendre transform (3.3.2) is invertible. Before proceeding (3.3.2) is put in terms of the fiber derivative $\mathbb{F}L : TQ \to T^*Q$

$$\mathbb{F}L(g, v) = (g, D_2 L(g, v)) = (g, p).$$

The variation of S with respect to g yields

$$\delta g \implies \int_a^b [D_1 L(g, v) \cdot \delta g + \langle p, \delta \dot{g} \rangle] \, dt = 0.$$

Integration by parts and using the boundary conditions yields,

$$\int_a^b [D_1 L(g, v) \cdot \delta g - \langle \dot{p}, \delta g \rangle] \, dt = 0.$$

From this it follows that

$$\dot{p} = -D_1 L(g, v). \tag{3.3.3}$$

Equations (3.3.1)-(3.3.3) are a differential algebraic system of equations. However, they can be viewed as an initial value problem with the following definition.

Definition 3.3.1. *The* ***allowable initial condition space*** $\mathcal{I}_{HP}$ *is defined to be the subset of* $TG \oplus T^*G$ *that satisfies (3.3.2), i.e.,*

$$\mathcal{I}_{HP} = \{(g, v, p) \in TG \oplus T^*G \mid p = D_2 L(g, v)\}.$$

Given an initial $(g(a), v(a), p(a)) \in \mathcal{I}_{HP}$ and a time interval $[a, b]$, one determines the point at b, $(g(b), v(b), p(b)) \in \mathcal{I}_{HP}$, by eliminating v using the Legendre transform (3.3.2) and solving the ODEs (3.3.1) and (3.3.3) for g and p. Let this map on $\mathcal{I}_{HP}$ be called the *HP flow map* and denoted by $F_{HP} : \mathcal{I}_{HP} \to \mathcal{I}_{HP}$.

The *natural projection* is denoted by $\pi_{HP} : TG \oplus T^*G \to T^*G$ and defined as,

$$\pi_{HP}(g, v, p) = (g, p).$$

Through π_{HP} the HP flow is identical to the Hamiltonian flow for the Hamiltonian of this mechanical system on T^*G obtained via the Legendre transformation. Although π_{HP} is not a diffeomorphism from $TG \oplus T^*G$ to T^*G, it is a diffeomorphism when its domain is restricted to $\mathcal{I}_{HP}$. It will be helpful to explicitly define this restriction as $\pi_{\mathcal{I}_{HP}} = \pi_{HP}|_{\mathcal{I}_{HP}}$. One can then write

$$\pi^{-1}_{\mathcal{I}_{HP}}(g, p) = (g, v, p), \quad (g, v) = \mathbb{F}L^{-1}(g, p).$$

As a consequence $TG \oplus T^*G$ is a presymplectic manifold with the *HP presymplectic form*, $\Omega_{HP} = \pi^*_{HP}\Omega$. Presymplectic means that the two-form is closed, but possibly degenerate. However, $\mathcal{I}_{HP}$ is a symplectic manifold with the *HP symplectic form*, $\Omega_{\mathcal{I}_{HP}} = \pi^*_{\mathcal{I}_{HP}}\Omega$. In the sequel we prove that the HP flow map preserves a momentum map and the symplectic form $\Omega_{\mathcal{I}_{HP}}$.

3.4 Unreduced HP Momentum Map

The *left action* of the Lie group on itself is denoted $\Phi : G \times G \to G$; that is, $\Phi(h, g) = L_h g = hg$. The natural *HP lift* of this action is likewise denoted $\Phi^{TG\oplus T^*G} : G \times (TG \oplus T^*G) \to TG \oplus T^*G$:

$$\begin{aligned}\Phi^{TG\oplus T^*G}(h, g, v, p) &= \left(\Phi(h, g), D_g\Phi(h, g) \cdot v, ((D_g\Phi(h, g))^{-1})^* \cdot p\right) \\ &= \left(L_h g, TL_h v, TL^*_{h^{-1}} p\right).\end{aligned}$$

For $x \in \mathfrak{g}$, define the map $\Phi_s^{TG\oplus T^*G} : \mathbb{R} \times (TG \oplus T^*G) \to TG \oplus T^*G$

$$\Phi_s^{TG\oplus T^*G}(g, v, p) = \Phi^{TG\oplus T^*G}(\exp(sx), g, v, p).$$

The corresponding *infinitesimal generator* $\psi^{TG\oplus T^*G} : TG \oplus T^*G \to T(TG \oplus T^*G)$ is by definition

$$\psi^{TG\oplus T^*G}(g, v, p) = \frac{d}{ds}\left[\Phi_s^{TG\oplus T^*G}(g, v, p)\right]_{s=0} = (xg, xv, -x^*p).$$

This action gives rise to the following momentum map $J : TG \oplus T^*G \to \mathfrak{g}^*$

$$J(g, v, p) \cdot x = \langle p, TR_g x\rangle = \left\langle TR_g^* p, x\right\rangle = \langle pg, x\rangle$$

where pg is understood as the right action of g on p. J is the standard cotangent momentum map for the second factor in the sum $TG \oplus T^*G$. The following conservation law follows from infinitesimal invariance of S.

Theorem 3.4.1 (**Conservation of HP momentum map**). *If S is infinitesimally symmetric, then the HP momentum map is conserved, i.e., $J = pg \cdot x$, is a conserved quantity under the HP flow.*

It is important to point out that infinitesimal invariance of S follows from left-invariance of the Lagrangian as follows. Left-invariance of the Lagrangian implies S is left-invariant because the first term in S is the Lagrangian itself and the second term is invariant with respect to the group action since

$$\langle hp, h\dot{g} - hv\rangle = \left\langle p, h^{-1}h(\dot{g} - v)\right\rangle = \langle p, \dot{g} - v\rangle .$$

Left invariance of the action integral implies that S is invariant with respect to the action of G on the space of curves given by pointwise action, i.e.,

$$S(g, v, p) = S \circ \Phi_s^{\mathcal{C}(TG\oplus T^*G)}(g, v, p), \tag{3.4.1}$$

where $\Phi_s^{\mathcal{C}(TG\oplus T^*G)} : \mathcal{C}(TG \oplus T^*G) \to \mathcal{C}(TG \oplus T^*G)$ given by

$$\Phi_s^{\mathcal{C}(TG\oplus T^*G)}(g, v, p)(t) = \Phi_s^{TG\oplus T^*G}(g(t), v(t), p(t)),$$

with infinitesimal generator given by

$$\psi^{\mathcal{C}(TG\oplus T^*G)}(g, v, p)(t) = \psi^{TG\oplus T^*G}(g(t), v(t), p(t)).$$

Differentiating (3.4.1) with respect to s using the chain rule and setting $s = 0$ gives the condition of infinitesimal invariance,

$$dS \cdot \psi^{\mathcal{C}(TG\oplus T^*G)}(g, v, p) = 0.$$

Proof. The *solution space*, $\mathcal{C}_{HP}(TG \oplus T^*G) \subset \mathcal{C}(TG \oplus T^*G)$, consists of elements of path space that are solutions to the HP variational principle. Consider the restriction of S to solution space: $\hat{S}$. Since a solution to the HP equations (or principle) for all $t \in [a, b]$ is uniquely determined by an initial $(g(a), v(a), p(a)) \in \mathcal{I}_{HP}$, solution space can be identified with the finite-dimensional manifold $\mathcal{I}_{HP}$, and hence, $\hat{S} : \mathcal{I}_{HP} \to \mathbb{R}$.

By integration by parts, one can write the differential of the restricted action integral as

$$\begin{aligned} &d\hat{S} \cdot \psi^{TG\oplus T^*G}(g(a), v(a), p(a)) \\ &\quad = \int_a^b \left[(D_1 L(g, v) - \dot{p}) \cdot xg + (D_2 L(g, v) - p) \cdot xv - (\dot{g} - v) \cdot x^* p\right] dt + \left.\langle p, xg\rangle\right|_a^b . \end{aligned}$$

Since this action integral is restricted to solution space the first three terms in the above vanish leaving the boundary terms. Moreover infinitesimal symmetry implies that

$$\begin{aligned} d\hat{S} \cdot \psi^{TG\oplus T^*G}(g(a), v(a), p(a)) &= 0, \\ \implies (F_{HP})^* J(g(a), v(a), p(a)) \cdot x - J(g(a), v(a), p(a)) \cdot x &= 0, \end{aligned}$$

and hence J is conserved under the HP flow. ■

3.5 Unreduced HP Symplectic Form

We define the *HP one-form*, $\Theta_{\mathcal{I}_{HP}} = \pi^*_{\mathcal{I}_{HP}}\Theta$, as the pullback of the canonical one-form under the map $\pi_{\mathcal{I}_{HP}}$. The differential of $\hat{S}$ can be written in terms of the HP one-form,

$$d\hat{S} \cdot (\delta g(a), \delta v(a), \delta p(a)) = \langle p, \delta g \rangle|_a^b = ((F_{HP})^* \Theta_{\mathcal{I}_{HP}} - \Theta_{\mathcal{I}_{HP}}) \cdot (\delta g(a), \delta v(a), \delta p(a)).$$

From the second differential of $\hat{S}$, one can show that F_{HP} defines a symplectic transformation on $\mathcal{I}_{HP}$.

Specifically, since $d^2\hat{S} = 0$, and since the pullback and d commute,

$$d^2\hat{S} = (F_{HP})^* \Omega_{\mathcal{I}_{HP}} - \Omega_{\mathcal{I}_{HP}} = 0,$$

where $\Omega_{\mathcal{I}_{HP}} = d\Theta_{\mathcal{I}_{HP}}$. Hence,

Theorem 3.5.1. *HP flows preserve the symplectic two-form* $\Omega_{\mathcal{I}_{HP}}$.

3.6 Reduced HP Flow

We now consider properties of solutions to the reduced HP principle. From the reduced HP principle, the variations of s with respect to ξ and μ give

$$\delta\mu \implies \xi = g^{-1}\dot{g}, \quad \text{(reconstruction equation)}, \tag{3.6.1}$$

$$\delta\xi \implies \mu = \ell'(\xi), \quad \text{(reduced Legendre transform)}. \tag{3.6.2}$$

Observe that in the reduced context, as is customary, we call the kinematic constraint the reconstruction equation. The variation of s with respect to g gives

$$\delta g \implies \int_a^b \left[\left\langle \mu, \delta(g^{-1}\dot{g})\right\rangle\right] dt = \int_a^b \left[\left\langle \mu, -g^{-1}\delta g g^{-1}\dot{g} + g^{-1}\delta\dot{g}\right\rangle\right] dt = 0.$$

Let $\eta = g^{-1}\delta g$. Using the product rule and (3.6.1), it is clear that

$$\frac{d}{dt}\eta = -\xi\eta + g^{-1}\frac{d}{dt}\delta g \implies g^{-1}\frac{d}{dt}\delta g = \frac{d}{dt}\eta + \xi\eta.$$

Substituting this relation into the above gives

$$\delta g \implies \int_a^b \left[\left\langle \mu, \frac{d}{dt}\eta + \operatorname{ad}_\xi \eta \right\rangle \right] dt = 0.$$

Integration by parts and using the boundary conditions on g yields

$$\int_a^b \left[\left\langle -\frac{d}{dt}\mu + \operatorname{ad}^*_\xi \mu, \eta \right\rangle \right] dt = 0.$$

Since the variations are arbitrary, one arrives at the LP equation.

$$\frac{d}{dt}\mu = \operatorname{ad}^*_\xi \mu, \quad \text{(LP equation)}. \tag{3.6.3}$$

(3.6.1)-(3.6.3) describe an IVP on the reduced space $G \times \mathfrak{g} \times \mathfrak{g}^*$. As in the unreduced case, we make this statement precise with the following definition.

Definition 3.6.1. *Let $\mathcal{I}_{hp}$ denote the* ***reduced allowable initial condition space*** *and defined as the subset of $G \times \mathfrak{g} \times \mathfrak{g}^*$ that satisfies (3.6.2), i.e.,*

$$\mathcal{I}_{hp} = \{(g, \xi, \mu) \in G \times \mathfrak{g} \times \mathfrak{g}^* \mid \mu = \ell'(\xi)\}. \tag{3.6.4}$$

Given a time-interval $[a, b]$ and an initial $(g(a), \xi(a), \mu(a)) \in \mathcal{I}_{hp}$, one can solve for $(g(b), \xi(b), \mu(b)) \in \mathcal{I}_{hp}$ by eliminating ξ using the reduced Legendre transform (3.6.2) and solving the ODEs (3.6.1) and (3.6.3) for g and μ. Let this map on $\mathcal{I}_{hp}$ be called the *reduced HP flow map*, $F_{hp} : \mathcal{I}_{hp} \to \mathcal{I}_{hp}$. This map is reduced since the ODEs (3.6.1) and (3.6.3) are decoupled, and hence, one can solve the LP equation (3.6.3) on $\mathfrak{g}^*$ independently from the reconstruction equation (3.6.1). Alternatively, one could eliminate μ using (3.6.2), to obtain the EP equation (1.1.2)

The reduced HP flow is equivalent to the HP flow on $\mathcal{I}_{HP}$ through left trivialization which defines a diffeomorphism between $TG \oplus T^*G$ and $G \times \mathfrak{g} \times \mathfrak{g}^*$, and hence, between $\mathcal{I}_{HP}$ and $\mathcal{I}_{hp}$. Thus, the reduced HP, HP and Hamiltonian flows of this mechanical system are all equivalent. This observation makes the subsequent development on proving momentum map preservation and symplecticity seem superfluous, since this structure obviously follows from the standard theory of Hamiltonian systems with symmetry. However, this verification is still important since it serves as a model for the less obvious discrete theory.

The manifold $G \times \mathfrak{g} \times \mathfrak{g}^*$ is a presymplectic manifold with the presymplectic form ω_{HP} that is obtained by pulling back the HP presymplectic form by the left trivialization of $TG \oplus T^*G$, $\phi : G \times \mathfrak{g} \times \mathfrak{g}^* \to TG \oplus T^*G$, i.e., $\omega_{HP} = \phi^* \Omega_{HP}$. However, as in the unreduced case, if the left-trivialization is restricted to $\mathcal{I}_{hp}$, $\phi_{\mathcal{I}_{hp}} = \phi|_{\mathcal{I}_{hp}}$, then $\mathcal{I}_{hp}$ is a symplectic manifold with the symplectic form given by $\omega_{\mathcal{I}_{hp}} = \phi^*_{\mathcal{I}_{hp}} \Omega_{\mathcal{I}_{HP}}$.

3.7 Reduced HP Momentum Map

The action of G on $G \times \mathfrak{g} \times \mathfrak{g}^*$ can be written in terms of the left action as,

$$\Phi^{G\times\mathfrak{g}\times\mathfrak{g}^*}(h, g, \xi, \mu) = (\Phi(h, g), \xi, \mu) \,. \tag{3.7.1}$$

For $x \in \mathfrak{g}$, define the map $\Phi_s^{G\times\mathfrak{g}\times\mathfrak{g}^*} : \mathbb{R} \times (G \times \mathfrak{g} \times \mathfrak{g}^*) \to G \times \mathfrak{g} \times \mathfrak{g}^*$

$$\Phi_s^{G\times\mathfrak{g}\times\mathfrak{g}^*}(g, \xi, \mu) = \Phi^{G\times\mathfrak{g}\times\mathfrak{g}^*}(\exp(sx), g, \xi, \mu).$$

The corresponding infinitesimal generator $\psi^{G\times\mathfrak{g}\times\mathfrak{g}^*} : G \times \mathfrak{g} \times \mathfrak{g}^* \to T(G \times \mathfrak{g} \times \mathfrak{g}^*)$ is, by definition,

$$\psi^{G\times\mathfrak{g}\times\mathfrak{g}^*}(g, \xi, \mu) = \frac{d}{ds}\left[\Phi_s^{G\times\mathfrak{g}\times\mathfrak{g}^*}(g, \xi, \mu)\right]_{s=0} = (xg, 0, 0). \tag{3.7.2}$$

This action gives rise to the following momentum map $J : G \times \mathfrak{g} \times \mathfrak{g}^* \to \mathfrak{g}^*$

$$J(g, \xi, \mu) \cdot x = \left\langle \operatorname{Ad}^*_{g^{-1}} \mu, x \right\rangle . \tag{3.7.3}$$

The following conservation law follows from the G-symmetry.

Theorem 3.7.1 (**Conservation of reduced HP momentum map**). *The reduced HP flow preserves the momentum map associated with the G-symmetry, namely $J = \mathrm{Ad}^*_{g^{-1}} \mu$.*

Proof. Infinitesimal symmetry of the reduced action integral is straightforward to check,

$$ds \cdot \psi^{\mathcal{C}(G\times\mathfrak{g}\times\mathfrak{g}^*)}(g,\xi,\mu) = \int_a^b \left[\left\langle \mu, \frac{d}{dt}(g^{-1}xg) + \mathrm{ad}_\xi\, g^{-1}xg \right\rangle\right] dt = 0$$

where $\psi^{\mathcal{C}(G\times\mathfrak{g}\times\mathfrak{g}^*)}$ is the infinitesimal generator associated with the action of G on $\mathcal{C}(G\times\mathfrak{g}\times\mathfrak{g}^*)$ given by pointwise action, i.e.,

$$\Phi_s^{\mathcal{C}(G\times\mathfrak{g}\times\mathfrak{g}^*)}(g,\xi,\mu)(t) = \Phi_s^{G\times\mathfrak{g}\times\mathfrak{g}^*}(g(t),\xi(t),\mu(t)).$$

Consider restricting the reduced HP action integral to the reduced solution space, $\hat{s} : \mathcal{I}_{hp} \to \mathbb{R}$. By integration by parts, one can write the differential of the restricted and reduced action integral as,

$$d\hat{s} \cdot \psi^{G\times\mathfrak{g}\times\mathfrak{g}^*}(g(a),\xi(a),\mu(a)) = \int_a^b \left[\left(-\frac{d\mu}{dt} + \mathrm{ad}^*_\xi\, \mu\right) \cdot \mathrm{Ad}_{g^{-1}}\, x\right] dt + \left\langle \mu, \mathrm{Ad}_{g^{-1}}\, x\right\rangle\Big|_a^b .$$

Since this action integral is restricted to solution space the first term vanishes. Moreover, infinitesimal symmetry implies that

$$d\hat{s}\cdot\psi^{G\times\mathfrak{g}\times\mathfrak{g}^*}(g(a),\xi(a),\mu(a)) = (F_{hp})^* J(g(a),\xi(a),\mu(a))\cdot x - J(g(a),\xi(a),\mu(a))\cdot x = 0$$

where $J = \mathrm{Ad}^*_{g^{-1}} \mu$ is the reduced HP momentum map (spatial angular momentum). And hence J is conserved under the reduced HP flow. ■

3.8 Reduced HP Symplectic Form

Again this structure of reduced HP flows is obvious from the standard theory of Hamiltonian systems with symmetry, but reviewing the proof will help since it parallels the discrete case.

As before the differential of $\hat{s}$ can be written as,

$$\begin{aligned} d\hat{s}\cdot(\delta g(a),\delta\xi(a),\delta\mu(a)) &= \int_a^b \left[\left(g^{-1}\dot{g}-\xi\right)\cdot\delta\mu(t)+\left(\mu-\ell'(\xi)\right)\cdot\delta\xi(t)\right]\,dt \\ &\quad+\int_a^b\left[\left(-\frac{d}{dt}\mu+\operatorname{ad}_\xi \mu\right)\cdot g^{-1}\delta g(t)\right]\,dt+\left\langle \mu, g^{-1}\delta g\right\rangle\Big|_a^b \\ &= \left\langle \mu, g^{-1}\delta g\right\rangle\Big|_a^b = ((F_{hp})^*\theta_{\mathcal{I}_{hp}}-\theta_{\mathcal{I}_{hp}})\cdot(\delta g(a),\delta\xi(a),\delta\mu(a)), \end{aligned}$$

where we have introduced the reduced HP one-form, $\theta_{\mathcal{I}_{hp}} = \phi^*_{\mathcal{I}_{hp}}\Theta_{\mathcal{I}_{HP}}$. Since $d^2\hat{s}=0$, observe that

$$d^2\hat{s} = (F_{hp})^*\omega_{\mathcal{I}_{hp}} - \omega_{\mathcal{I}_{hp}} = 0.$$

And hence, as a map on $\mathcal{I}_{hp}$, F_{hp} is a symplectic map.

Theorem 3.8.1. *Reduced HP flows preserve the symplectic two-form* $\omega_{\mathcal{I}_{hp}}$.

Chapter 4

HP Integrator for EP Systems

In this chapter a discrete, reduced HP description of mechanics is introduced. The configuration space is assumed to be a finite-dimensional Lie group. This chapter parallels the VPRK theory on vector spaces with one main exception: the chapter begins with a discussion of local coordinates on a Lie group. A discretization for the reconstruction equation based on Runge-Kutta-Munthe-Kaas methods is suggesed. However, in this chapter only an Euler-Munthe-Kaas discretization is built into an action sum using Lagrange multipliers. The reader is referred to the future directions chapter for the general case.

4.1 Canonical Coordinates of the First Kind

To setup the discrete HP principle, we introduce a map $\tau : \mathfrak{g} \to G$. Let $e \in G$ be the identity element of the group. The map τ is assumed to be a local diffeomorphism mapping a neighborhood of zero on $\mathfrak{g}$ to one of e on G with $\tau(0) = e$, and assumed to be analytic in this neighborhood. Thereby τ provides a local chart on the Lie group. By left translation this map can be used to construct an atlas on G. For our purposes τ can be regarded as an approximant to the exponential map on G.

Definition 4.1.1. *The local coordinates associated with the map τ are called **canonical coordinates of the first kind** or just **canonical coordinates**.*

For an exposition of canonical coordinates of the first and second kind, and their applications the reader is referred to [19]. In what follows we will prove some properties of these coordinates that will be needed shortly. The most basic is the following.

Lemma 4.1.2. *If $\tau : \mathfrak{g} \to G$ is a local diffeomorphism and analytic, then $\tau(\xi) \cdot \tau(-\xi) = e$.*

Proof. Since τ is a local diffeomorphism there exists some ball $\mathcal{B}_r \subset \mathfrak{g}$ defined as

$$\mathcal{B}_r = \{x \in \mathfrak{g} \mid \|x\| \leq r\}$$

in which $\tau|_V : V \to \tau(V) \subset G$ is a diffeomorphism.

Consider $\xi \in V$ and define:

$$f(t) = \tau(t\xi)\tau(-t\xi), \quad t \in [0, 1].$$

Observe that $f(0) = e$ and since τ is analytic,

$$\frac{d}{dt} f(t) = TL_{\tau(t\xi)} TR_{\tau(-t\xi)}\xi - TL_{\tau(t\xi)} TR_{\tau(-t\xi)}\xi = 0.$$

Therefore f is constant and,

$$f(1) = \tau(\xi)\tau(-\xi) = e.$$

■

Derivative of $\boldsymbol{\tau}$ and its inverse. To derive the integrator that comes from a discrete reduced HP principle, we will need to differentiate τ^{-1}. The *right trivialized tangent* of τ and its inverse will play an important role in writing this derivative in an efficient way. The definition of τ is based on definition 2.19 in [19].

Definition 4.1.3. *Given a local diffeomorphism $\tau : \mathfrak{g} \to G$, we define its* ***right***

trivialized tangent *to be the function* $d\tau : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ *which satisifies,*

$$\mathrm{D}\,\tau(\xi) \cdot \delta = TR_{\tau(\xi)} d\tau_{\xi}(\delta).$$

The function $d\tau$ *is linear in its second argument.*

Fig. 4.1.2 illustrates the geometry behind this definition. It shows that the right trivialized tangent is (as the name suggests) the differential of τ applied to a tangent vector at the identity and then right trivialized back to the tangent space at the identity. This operation gives a well-defined and invertible map since τ is assumed to be a local diffeomorphism.

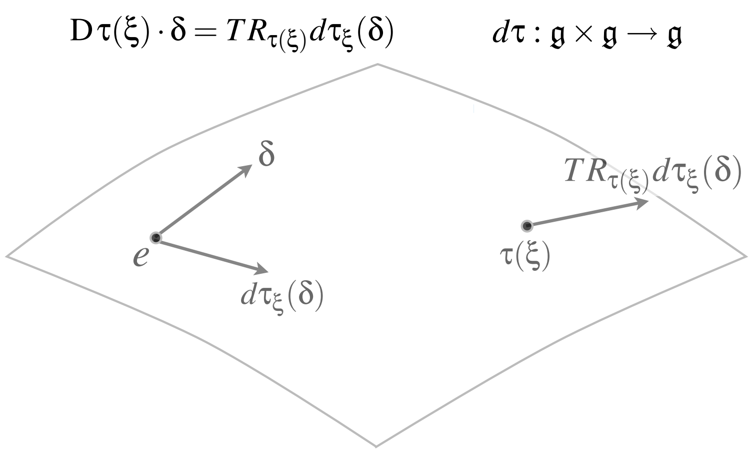


Figure 4.1.1: **Derivative of τ.** Definition (4.1.3) splits the differential of τ into a map on the Lie algebra (the right trivialized tangent of τ) and right multiplication to the tangent space at $\tau(\xi)$.

From this definition the following lemma is deduced.

Lemma 4.1.4. *The following identity holds,*

$$d\tau_{\xi}(\delta) = \mathrm{Ad}_{\tau(\xi)}\, d\tau_{-\xi}(\delta).$$

Proof. Differentiation of $\tau(\xi) \cdot \tau(-\xi) = e$ implies that,

$$\mathrm{D}\,\tau(-\xi) \cdot \delta = -TL_{\tau(-\xi)} TR_{\tau(-\xi)} \left(\mathrm{D}\,\tau(\xi) \cdot \delta\right).$$

While the chain rule implies that,

$$\mathrm{D}\,\tau(-\xi) \cdot \delta = -TR_{\tau(-\xi)} d\tau_{-\xi}(\delta).$$

Combining these two identities and using the definition above,

$$-TR_{\tau(-\xi)} d\tau_{-\xi}(\delta) = -TL_{\tau(-\xi)} TR_{\tau(-\xi)} TR_{\tau(\xi)} d\tau_{\xi}(\delta).$$

Simplifying this expression gives,

$$TL_{\tau(\xi)} d\tau_{-\xi}(\delta) = TR_{\tau(\xi)} d\tau_{\xi}(\delta).$$

This proves the identity. ■

We will also need a simple expression for the differential of τ^{-1}.

Definition 4.1.5. *The* ***inverse right trivialized tangent*** *of τ is the function $d\tau^{-1} : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ which satisifies for $g = \tau(\xi)$,*

$$\mathrm{D}\,\tau^{-1}(g) \cdot \delta = d\tau_{\xi}^{-1}(TR_{\tau(-\xi)}\delta), \quad d\tau_{\xi}^{-1}(d\tau_{\xi}(\delta)) = \delta.$$

The function $d\tau^{-1}$ is always linear in its second argument.

Fig. 4.1.2 illustrates the geometry behind this definition. The inverse right trivialized tangent is obtained by applying the differential of τ^{-1} to a tangent vector at the identity right translated to $\tau(\xi) \in G$.

The following lemma follows from this definition and lemma 4.1.4 above.

Lemma 4.1.6. *The following identity holds,*

$$d\tau_{\xi}^{-1}(\delta) = d\tau_{-\xi}^{-1}(\mathrm{Ad}_{\tau(-\xi)}\,\delta).$$

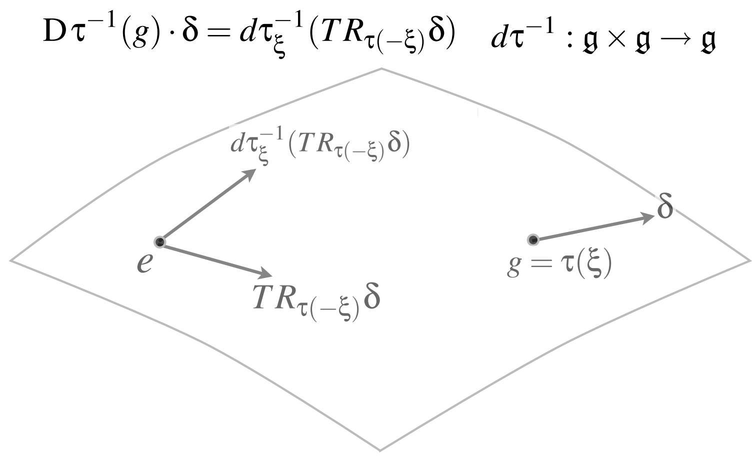


Figure 4.1.2: **Derivative of τ^{-1}.** Definition (4.1.5) splits the differential of τ^{-1} into right multiplication to the Lie algebra and a map on the Lie algebra (the right trivialized tangent of τ^{-1}).

Proof. This follows directly from lemma 4.1.4. Let $\delta \to d\tau_{\xi}^{-1}(\delta)$ in that identity to obtain

$$\delta = \mathrm{Ad}_{\tau(\xi)}\, d\tau_{-\xi}(d\tau_{\xi}^{-1}(\delta)).$$

And now solve this equation for $d\tau_{\xi}^{-1}(\delta)$,

$$d\tau_{\xi}^{-1}(\delta) = d\tau_{-\xi}^{-1}\left(\mathrm{Ad}_{\tau(-\xi)}\,\delta\right).$$

■

The final lemma will be important in analyzing the local and global error of the VPRK methods we intend to design.

Lemma 4.1.7. *Assume that $\tau(\xi)$ is a qth order approximant to the exact exponential map. Then $d\tau_{\xi}$ and $d\tau_{\xi}^{-1}$ are also qth order approximants to $d\exp_{\xi}$ and $d\exp_{\xi}^{-1}$, respectively.*

Proof. If $\tau(\xi)$ is a qth order approximant to the exact exponential map, then one can write,

$$\tau(\xi) = \exp(\xi) + \mathcal{O}(h^q). \tag{4.1.1}$$

From which it follows that

$$\exp(\xi)\tau(-\xi) = e + \mathcal{O}(h^q).$$

where e is the identity element of the group. Differentiating (4.1.1) in the direction δ gives

$$TR_{\tau(\xi)} d\tau_\xi \delta = TR_{\exp(\xi)} d\exp_\xi \delta + \mathcal{O}(h^q) \implies d\tau_\xi \delta = TR_{\exp(\xi)\tau(-\xi)} d\exp_\xi \delta + \mathcal{O}(h^q).$$

Using (4.1.1) one can simplify this expression to,

$$d\tau_\xi \delta = d\exp_\xi \delta + \mathcal{O}(h^q).$$

The transformation $\delta \mapsto d\tau_\xi^{-1}\delta$ provides the corresponding order condition for $d\tau_\xi^{-1}$. ■

4.2 RKMK Discrete Reconstruction Equation

Let $[a, b]$ and N be given, let $h = (b - a)/(N - 1)$ be a fixed integration time step and $t_k = hk$. A good candidate for discretizing the reconstruction equation is given by a generalization of s-stage Runge-Kutta methods to differential equations on Lie groups, namely Runge-Kutta-Munthe-Kaas (RKMK) methods introduced in the following series of papers [40; 43; 41; 42]. The idea behind those papers is to use canonical coordinates on the Lie group to transform the differential equation on TG, e.g., given by,

$$\dot{g} = TL_g f(t, g), \quad g(0) = g_0, \quad g(t) \in G, \quad f(t, g(t)) \in \mathfrak{g}, . \tag{4.2.1}$$

to a differential equation on $\mathfrak{g}$. Specifically, introduce the following parametrization $g(t) = g_0\tau(\Theta(t))$ and substitute it into (4.2.1) to obtain,

$$\dot{g} = TR_{g_0}TR_{\tau(\Theta)}d\tau_\Theta\dot{\Theta} = TR_{g_0}TL_{\tau(\Theta)}f(t,g).$$

Using lemma 4.1.4 this equation can be rewritten as,

$$TL_{\tau(-\Theta)}TR_{\tau(\Theta)}d\tau_\Theta\dot{\Theta} = \mathrm{Ad}_{\tau(-\Theta)}\, d\tau_\Theta\dot{\Theta} = d\tau_{-\Theta}\dot{\Theta} = f(t,g).$$

Solving for $\dot{\Theta}$ gives

$$\dot{\Theta} = d\tau_{-\Theta}^{-1}f(t,g), \quad \Theta(0) = 0, \quad \Theta(t) \in \mathfrak{g}. \tag{4.2.2}$$

As described in the following definition, the RKMK method is obtained by applying an s-stage Runge-Kutta method to (4.2.2) with a suitable reconstruction procedure.

Definition 4.2.1. *Consider the first-order differential equation $\dot{g} = f(t,g)$ for $(g(t), f(t,g(t))) \in TG$ and let $b_i, a_{ij} \in \mathbb{R}$ $(i,j = 1,\cdots,s)$ and let $c_i = \sum_{j=1}^s a_{ij}$. An* ***s-stage Runge-Kutta-Munthe-Kaas*** *(RKMK) approximation is given by*

$$G_k^i = \tau(\Theta_k^i)g_k, \quad \Theta_k^i = h\sum_{j=1}^s a_{ij}d\tau_{-\Theta_k^j}^{-1}\left(f(t_k + c_jh, G_k^j)\right), \quad i = 1,\cdots,s, \tag{4.2.3}$$

$$g_{k+1} = g_k\tau\left(h\sum_{j=1}^s b_jf(t_k + c_jh, G_k^j)\right). \tag{4.2.4}$$

If $a_{ij} = 0$ for $i \le j$ the RKMK method is called explicit, and implicit otherwise. The vectors g_k and G_k^i are called external and internal stage configurations, respectively.

From this definition it is clear that an s-stage RKMK method applied to the reconstruction equation can be written as:

$$\Theta_k^i/h = \sum_{j=1}^{s} a_{ij} d\tau^{-1}_{-\Theta_k^j} \Xi_k^j, \quad i = 1, \cdots, s, \tag{4.2.5}$$

$$\tau^{-1}(g_k^{-1} g_{k+1})/h = \sum_{i=1}^{s} b_i \Xi_k^i, \tag{4.2.6}$$

where $\Xi_k^i = \xi(t_k + c_i h)$. In practice one truncates the series expansion of $d\tau^{-1}_{-\Theta_k^j}$. The following theorem guides how to do this without wrecking the order of accuracy.

Theorem 4.2.2. *Suppose that τ is a qth order approximant to the exact exponential. If the RKMK method is of order p and the truncation index of $d\tau^{-1}_{-\Theta_k^j}$ satisfies $q \geq p - 2$ then the RKMK method is of order p.*

Proof. This theorem is a simple extension of a property of RKMK methods to account for the fact that τ is not the exponential map exactly [15]. ■

4.3 Discrete Reduced HP Principle

Definition 4.3.1. *Define the* ***discrete reduced path space****,*

$$\mathcal{C}_d(G \times \mathfrak{g} \times \mathfrak{g}^*) = \{(g, \xi, \mu)_d \mid \{t_k\}_{k=0}^N \to G \times \mathfrak{g} \times \mathfrak{g}^*\}.$$

and the ***reduced action sum*** $s_d : \mathcal{C}_d(G \times \mathfrak{g} \times \mathfrak{g}^*) \to \mathbb{R}$ *as*

$$s_d(\{g_k, \xi_k, \mu_k\}_{k=0}^N) = \sum_{k=0}^{N-1} h \left[\ell(\xi_k) + \left\langle \mu_k, \tau^{-1}(g_k^{-1} g_{k+1})/h - \xi_k \right\rangle \right]. \tag{4.3.1}$$

The reduced action sum, s_d, is an approximation of the reduced action integral by numerical quadrature. The definition of τ as a map from $\mathfrak{g}$ to G ensures that the second term as a pairing on the Lie algebra is well defined. The discrete reduced HP principle states that,

$$\delta s_d = 0$$

for arbitrary and independent variations of $(g_k, \xi_k, \mu_k) \in G \times \mathfrak{g} \times \mathfrak{g}^*$ subject to fixed endpoint conditions on $\{g_k\}_{k=0}^N$.

4.4 Derivation from HP Action Sum

Here the reduced HP action sum will be derived from an approximation of the HP action integral. First an approximation of TG that yields a single-step scheme on phase space will be introduced.[1] We introduce the discretization map $\varphi : G \times G \to TG$ which defines the discrete approximation of TG by $G \times G$. This map is defined in terms of approximants to the current configuration $g(t) \in G$ and body angular velocity $\xi(t) \in \mathfrak{g}$, given by the functions $\kappa : G \times G \to G$ and $\Gamma : G \times G \to \mathfrak{g}$ as follows,

$$\varphi(g_k, g_{k+1}) = (\kappa(g_k, g_{k+1}), T_e L_{\kappa(g_k, g_{k+1})} \Gamma(g_k, g_{k+1})).$$

The discrete Lagrangian $L_d : G \times G \to \mathbb{R}$ is now designed in terms of the original Lagrangian and this discretization as,

$$L_d(g_k, g_{k+1}) = L \circ \varphi(g_k, g_{k+1}) = L(\kappa(g_k, g_{k+1}), T_e L_{\kappa(g_k, g_{k+1})} \Gamma(g_k, g_{k+1})).$$

The *discrete path space* is defined as,

$$\mathcal{C}_d(TG \oplus T^*G) = \{(g, v, p)_d : \{t_k\}_{k=0}^N \to TG \oplus T^*G\}.$$

In terms of the discretization defined by φ the HP action sum $S_d : \mathcal{C}_d(TG \oplus T^*G) \to \mathbb{R}$ can be written as,

$$\begin{aligned} S_d(\{g_k, v_k, p_k\}_{k=0}^N) = \sum_{k=0}^{N-1} h \big[& L(\kappa(g_k, g_{k+1}), TL_{\kappa(g_k, g_{k+1})} v_k) \\ & + \left\langle p_k, TL_{\kappa(g_k, g_{k+1})} \Gamma(g_k, g_{k+1}) - v_k \right\rangle \big] . \end{aligned}$$

[1] This discretization map was suggested by Alessandro Saccon who made this remark to us after reviewing an earlier version of this work.

However, left invariance of L implies that

$$
\begin{aligned}
&S_d(\{g_k, v_k, p_k\}_{k=0}^N) \\
&\quad = \sum_{k=0}^{N-1} h \left[L(e, \Gamma(g_k, g_{k+1})) + \left\langle TL^*_{\kappa(g_k,g_{k+1})} p_k, \Gamma(g_k, g_{k+1}) - TL_{\kappa(g_k,g_{k+1})^{-1}} v_k \right\rangle \right] \\
&\quad = \sum_{k=0}^{N-1} h \left[\ell(\Gamma(g_k, g_{k+1})) + \left\langle TL^*_{\kappa(g_k,g_{k+1})} p_k, \Gamma(g_k, g_{k+1}) - TL_{\kappa(g_k,g_{k+1})^{-1}} v_k \right\rangle \right].
\end{aligned}
$$

If Γ is left invariant, i.e.,

$$
\Gamma(hg_k, hg_{k+1}) = \Gamma(g_k, g_{k+1}),
$$

for all $h \in G$, then this expression can be further simplified to,

$$
S_d(\{g_k, v_k, p_k\}_{k=0}^N) = \sum_{k=0}^{N-1} h \left[\ell(\Gamma(e, g_k^{-1} g_{k+1})) + \left\langle \mu_k, \Gamma(e, g_k^{-1} g_{k+1}) - \xi_k \right\rangle \right],
$$

where $\mu_k = TL^*_{\kappa(g_k,g_{k+1})} p_k$ and $\xi_k = TL_{\kappa(g_k,g_{k+1})^{-1}} v_k$. Now define $\tau^{-1}(g_k^{-1} g_{k+1})/h = \Gamma(e, g_k^{-1} g_{k+1})$ to obtain (4.3.1).

4.5 Example: Free Rigid Body on S^3

There are other discrete principles one could consider. For example, one could employ the Moser-Veselov approach of embedding the Lie group in a larger linear space and constraining to the group using Lagrange multipliers. This approach does not take advantage of the Lie group symmetry to accelerate the computation. These different choices are illustrated here in the context of the free rigid body on S^3.

Define the discrete Lagrangian of the free rigid body, $L_d : \mathbb{R}^4 \times \mathbb{R}^4 \to \mathbb{R}$, as an approximation to L that inherits the G-symmetry,

$$
L_d(g_k, g_{k+1}) = L_d(B \star g_k, B \star g_{k+1}),
$$

for all $B \in S^3$. Let $L_d^c : S^3 \times S^3 \to \mathbb{R}$ denote the constrained discrete Lagrangian defined as $L_d^c = L_d|_{S^3 \times S^3}$.

Let f_{kk+1} denote an element of the discrete reduced space $S^3 \times S^3/S^3$. Restricting L_d^c to this space gives the reduced discrete Lagrangian $\ell_d : S^3 \to \mathbb{R}$,

$$\ell_d(f_{kk+1}) = L_d^c(e, f_{kk+1}).$$

Form the reduced action sum,

$$s_{DEP} = \sum_{k=0}^{N-1} h\ell_d(f_{kk+1}).$$

Then the DEP principle states that

$$\delta s_{DEP} = 0$$

with respect to variations of f_{kk+1} that are no longer arbitrary, but induced by the group [35].

Alternatively one can derive a Moser-Veselov integrator as follows [39]. Consider the unconstrained action sum defined by,

$$S = \sum_{k=0}^{N-1} hL_d(g_k, g_{k+1}).$$

The constraint $\varphi(g_k) = 0$ is enforced by introducing a constrained action sum S_{MV} with the Lagrange multipliers $\{\lambda_k\}_{k=0}^{N-1}$,

$$S_{MV} = \sum_{k=0}^{N-1} h\left[L_d(g_k, g_{k+1}) + \lambda_k \varphi(g_k)\right].$$

S_{MV} defines the Moser-Veselov action sum. The Moser-Veselov variational principle is simply discrete Hamilton's principle with the holonomic constraint $\varphi(g_k) = 0$ enforced using Lagrange multipliers. This is precisely the approach laid out in [48]. The equivalence between the DEP and Moser-Veselov principles is a straightforward application of theorem 1 of that paper.

The reduced HP action sum can be written as

$$s_d = \sum_{k=0}^{N-1} h\left[\ell(\mathbf{\Omega}_k) + \left\langle \mathbf{\Pi}_k, \tau^{-1}(g_k^{-1} g_{k+1})/h - \mathbf{\Omega}_k \right\rangle\right].$$

An example of τ is given by the exponential from $\mathbb{R}^3$ to S^3. More precisely, for $\mathbf{\Omega} \in \mathbb{R}^3$ and $\theta = \sqrt{\mathbf{\Omega}^T \mathbf{\Omega}}$, $\tau : \mathbb{R}^3 \to S^3$ is given by

$$\tau(\mathbf{\Omega}) = (\cos(\theta/2), \sin(\theta/2)/\theta\mathbf{\Omega}).$$

4.6 Discrete Reduced HP Flow Map

The variation of s_d with respect to μ_k and ξ_k in the discrete reduced HP principle imply the following difference equations are satisfied for $k = 0, \cdots, N-1$,

$$\delta\mu_k \implies g_k^{-1} g_{k+1} = \tau(h\xi_k), \quad \text{(discrete reconstruction equation)}, \tag{4.6.1}$$

$$\delta\xi_k \implies \ell'(\xi_k) = \mu_k, \quad \text{(discrete, reduced Legendre transform)}. \tag{4.6.2}$$

The first equation is a discrete reconstruction equation which through the map τ relates $g_k^{-1} g_{k+1}$ to ξ_k. In this formulation it is a constraint equation with Lagrange multiplier being $\mu_k \in \mathfrak{g}^*$.

The variation of s_d with respect to g_k implies,

$$\delta g_k \implies \sum_{k=0}^{N-1} \left[\left\langle \mu_k, \delta\tau^{-1}(g_k^{-1} g_{k+1}) \right\rangle\right] = 0.$$

Defining $\eta_k = g_k^{-1} \delta g_k$, and using the chain rule, one can write the above as

$$\sum_{k=0}^{N-1} \left[\left\langle \mu_k, \mathrm{D}\,\tau^{-1}(\tau(h\xi_k)) \cdot (-TR_{\tau(h\xi_k)}\eta_k + TL_{\tau(h\xi_k)}\eta_{k+1}) \right\rangle\right] h = 0.$$

In terms of the inverse right trivialized tangent, this can be written as

$$\sum_{k=0}^{N-1} \left[\left\langle \mu_k, d\tau^{-1}_{h\xi_k}(-\eta_k + \mathrm{Ad}_{\tau(h\xi_k)}\, \eta_{k+1}) \right\rangle \right] h = 0.$$

Summation by parts, the boundary conditions $\delta g_0 = \delta g_N = 0$, and lemma 4.1.6 imply that this can be rewritten as

$$\sum_{k=1}^{N-1} \left[\left\langle \mu_k, d\tau^{-1}_{h\xi_k}(-\eta_k) \right\rangle + \left\langle \mu_{k-1}, d\tau^{-1}_{-h\xi_{k-1}}(\eta_k) \right\rangle \right] h = 0.$$

Factoring out η_k gives

$$\sum_{k=1}^{N-1} \left[\left\langle -(d\tau^{-1}_{h\xi_k})^* \mu_k + (d\tau^{-1}_{-h\xi_{k-1}})^* \mu_{k-1}, \eta_k \right\rangle \right] h$$

which implies the following difference equation holds,

$$(d\tau^{-1}_{h\xi_k})^* \mu_k = (d\tau^{-1}_{-h\xi_{k-1}})^* \mu_{k-1}, \quad \text{(discrete LP equation)}. \tag{4.6.3}$$

Together (4.6.1)-(4.6.3) define a HPVI, that is, an update scheme on $G \times \mathfrak{g} \times \mathfrak{g}^*$. (4.6.3) is statement of balance of momentum as illustrated in Fig. 4.6.1. If one eliminates μ_k using the reduced Legendre transform, one obtains the discrete EP equations.

For example, given $(g_k, \xi_k, \mu_k) \in \mathcal{I}_{hp}$ one determines $(g_{k+1}, \xi_{k+1}, \mu_{k+1}) \in \mathcal{I}_{hp}$ by eliminating ξ_k and ξ_{k+1} using (4.6.2) and then solving (4.6.3) for μ_{k+1} and (4.6.1) for g_{k+1}. Let N iterations of such an update procedure be called the *discrete reduced HP flow map*, $F^N_{hp} : \mathbb{Z} \times \mathcal{I}_{hp} \to \mathcal{I}_{hp}$.

The following examples evaluate (4.6.3) for various choices of τ.

Examples

(a) Matrix exponential. Suppose

$$\tau = \exp(\xi), \quad \tau : \mathfrak{g} \to G,$$

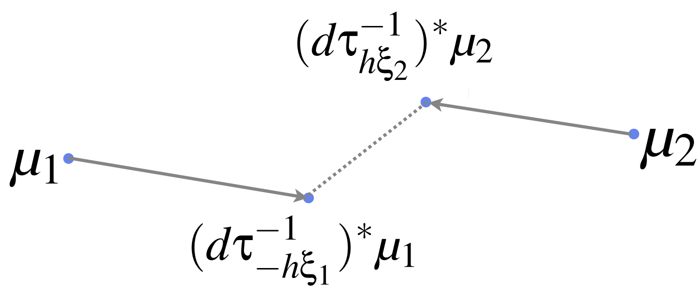


Figure 4.6.1: **HPVI balance of momentum.** This figure illustrates (4.6.3) when $k = 2$. The equality in (4.6.3)—a statement of balance of momentum from one timestep to the next—is represented by the dotted line.

which is a local diffeomorphism.

Using standard convention the right trivialized tangent of the exponential map and its inverse are denoted by $\text{dexp} : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ and $\text{dexp}^{-1} : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$, and are explicitly given by,

$$\text{dexp}(x)y = \sum_{j=0}^{\infty} \frac{1}{(j+1)!} \operatorname{ad}_x^j y, \quad \text{dexp}^{-1}(x)y = \sum_{j=0}^{\infty} \frac{B_j}{j!} \operatorname{ad}_x^j y, \tag{4.6.4}$$

where B_j are the *Bernoulli numbers* [15, see §3.4 for a detailed exposition/derivation].

Hence, (4.6.3) takes the form,

$$(\text{dexp}^{-1}(h\xi_k))^* \mu_k = (\text{dexp}^{-1}(-h\xi_{k-1}))^* \mu_{k-1}. \tag{4.6.5}$$

Together with (4.6.1) and (4.6.2), (4.6.5) defines the *exponential-based HPVI* (EXP). After eliminating μ_k using (4.6.2), (4.6.5) are the DEP equations in local coordinates given by the exponential map [35, See (4.12)].

(b) Padé (1,1) approximant. Suppose

$$\tau(\xi) = \text{cay}(\xi) = (e - \xi/2)^{-1}(e + \xi/2), \tag{4.6.6}$$

which is the Padé (1,1) approximant to the matrix exponential and better known as the *Cayley transform*. The Cayley transform maps to the group for quadratic Lie groups ($SO(n)$, the symplectic group $Sp(2n)$, the Lorentz group $SO(3,1)$) and the special Euclidean group $SE(3)$.

The right-trivialized tangent of the Cayley transform and its inverse are written below

$$\mathrm{dcay}(x)y = (e - x/2)^{-1} y (e + x/2)^{-1}, \quad \mathrm{dcay}^{-1}(x)y = (e - x/2) y (e + x/2). \tag{4.6.7}$$

For a derivation and exposition the reader is referred to §4.8.3 [15]. Using these expressions (4.6.3) can be written as,

$$\begin{aligned} \mu_k =& \mu_{k-1} + \frac{h}{2} \mathrm{ad}^*_{\xi_k} \mu_k + \frac{h}{2} \mathrm{ad}^*_{\xi_{k-1}} \mu_{k-1} \\ &+ \frac{h^2}{4} \left(\xi_k^* \mu_k \xi_k^* - \xi_{k-1}^* \mu_{k-1} \xi_{k-1}^* \right) \end{aligned} \tag{4.6.8}$$

which together with (4.6.1) and (4.6.2) defines the *Cayley-based HPVI* (CAY).

(c) Padé (1,0) or (0,1) approximant. Rather than use the exact matrix exponential one can use a Padé approximant, e.g., the Padé (1,0) approximant

$$\exp(\xi) \approx e + \xi$$

or Padé (0,1) approximant

$$\exp(\xi) \approx (e - \xi)^{-1}.$$

However, since a Padé approximant is not guaranteed to lie on the group one needs to use a projector from $GL(n)$ to G. In what follows $G = SO(n)$ will be considered where a natural choice of projector is given by skew symmetrization.

Suppose

$$\tau^{-1}(g) = \operatorname{skew}(g) = \frac{g - g^*}{2}.$$

which comes from a first order approximant to the matrix exponential. This map is a local diffeomorphism from a neighborhood of e to a neighborhood of 0 and its differential is the identity. Its right trivialized tangent can be computed from its derivative:

$$\mathrm{D}\operatorname{skew}(g) \cdot \delta = \frac{\delta - \delta^*}{2} = \frac{(\delta g^{-1} g) - (\delta g^{-1} g)^*}{2}.$$

By definition of the right trivialized tangent of τ^{-1}, it then follows that,

$$\operatorname{dskew}(x)(y) = \frac{y\tau(x) - (y\tau(x))^*}{2}. \tag{4.6.9}$$

Cardoso and Leite state and prove the following theorem that explicitly determines $\tau(\xi)$. Moreover, they give necessary and sufficient conditions for its existence [8].

Theorem 4.6.1. *Given $\xi \in \mathfrak{so}(\mathfrak{n})$, a special orthogonal solution to the equation*

$$\xi = \frac{\tau(\xi) - \tau(\xi)^*}{2}$$

can be written as

$$\tau(\xi) = \xi + \left(\xi^2 + e\right)^{1/2},$$

where $\left(\xi^2 + e\right)^{1/2}$ is a symmetric square root.

Proof. Since the skew-symmetric part of g is ξ, one can write g as a sum of ξ and a symmetric matrix S,

$$\tau(\xi) = S + \xi.$$

Observe that ξ commutes with $\tau(\xi)$ since

$$2\xi\tau(\xi) = (\tau(\xi) - \tau(\xi)^*)\tau(\xi) = \tau(\xi)^2 - e = 2\tau(\xi)\xi.$$

Moreover, S satisfies an algebraic Riccati equation because,

$$\tau(\xi)^*\tau(\xi) = e \implies S^2 + S\xi - \xi S - (\xi^2 + e) = 0.$$

And since ξ commutes with S (because it commutes with g),

$$S^2 = (\xi^2 + e),$$

which completes the proof. ■

Hence, (4.6.3) can be written as,

$$\begin{aligned} &\frac{\mu_k \left(h^2\xi_k^2 + e\right)^{1/2} + \left(h^2\xi_k^2 + e\right)^{1/2} \mu_k}{2} \\ &\quad = \frac{\mu_{k-1} \left(h^2\xi_{k-1}^2 + e\right)^{1/2} + \left(h^2\xi_{k-1}^2 + e\right)^{1/2} \mu_{k-1}}{2} \\ &\qquad + \frac{h}{2} \operatorname{ad}^*_{\xi_k} \mu_k + \frac{h}{2} \operatorname{ad}^*_{\xi_{k-1}} \mu_{k-1} \end{aligned} \tag{4.6.10}$$

4.7 Order of Accuracy

In this section the global error of the variational Euler integrator is examined.

To determine the order of accuracy of the reduced HP flow map one can invoke a theorem relating the order of accuracy of a discrete Lagrangian and corresponding discrete Legendre transform and Hamiltonian map [49, see theorem 3.3]. To use this theorem, one needs to write down the discrete Lagrangian associated with the reduced HP action sum. As demonstrated earlier the discrete Lagrangian is given by,

$$L_d(g_k, g_{k+1}) = \ell(\tau^{-1}(g_k^{-1} g_{k+1})) = L(e, \tau^{-1}(g_k^{-1} g_{k+1})).$$

This identity also suggests that one could replace the continuous reduced Lagrangian ℓ with a discrete approximation to it that is within the order of accuracy of the desired method. However, for simplicity we avoid introducing a more general modified ℓ in this paper.

Alternatively one can prove second-order global accuracy directly as is done below. We arrive at order conditions by comparing the Taylor expansion of the exact solution to (3.6.1)-(3.6.3) and the numerical approximant generated by a VPRK integrator. Suppose that $g_k = g(t_k)$, $\xi_k = \xi(t_k)$, and $\mu_k = \mu(t_k)$ are exact. Then the Taylor expansion of the exact solution about t_k for h small is given by:

$$\mu(t_k + h) = \mu_k + h \operatorname{ad}^*_{\xi_k} \mu_k + \frac{h^2}{2} \left(\operatorname{ad}^*_{\xi_k} \operatorname{ad}^*_{\xi_k} \mu_k + \operatorname{ad}_{\dot{\xi}_k} \mu_k \right) \\ + \frac{h^3}{6} \left(2 \operatorname{ad}^*_{\dot{\xi}_k} \operatorname{ad}^*_{\xi_k} \mu_k + \operatorname{ad}^*_{\xi_k} \operatorname{ad}^*_{\dot{\xi}_k} \mu_k + \operatorname{ad}^*_{\ddot{\xi}_k} \mu_k + \operatorname{ad}^*_{\xi_k} \operatorname{ad}^*_{\xi_k} \operatorname{ad}^*_{\xi_k} \mu_k \right) + \mathcal{O}(h^4),$$

and,

$$g(t_k + h) = g_k + h g_k \xi_k + \frac{h^2}{2} \left(g_k \xi_k^2 + g_k \dot{\xi}_k \right) \\ + \frac{h^3}{6} \left(g_k \xi_k^3 + g_k \dot{\xi}_k \xi_k + 2 g_k \xi_k \dot{\xi}_k + g_k \ddot{\xi}_k \right) + \mathcal{O}(h^4).$$

Using these expansions one can prove the following.

Theorem 4.7.1. *If τ is a second-order approximant to the exponential map, then the global error of the approximant to g and μ determined by (7.2.1) is of second-order.*

Proof. The Taylor expansion of the variational Euler approximant to $\mu(t_{k+1})$ given that $\mu_k = \mu(t_k)$ is exact, can be computed by regarding the approximant as a function of h and successively differentiating the difference scheme (7.2.1) to obtain:

$$\left. \frac{\partial \mu_{k+1}}{\partial h}(h) \right|_{h=0} = \operatorname{ad}^*_{\xi_k} \mu_k, \qquad \left. \frac{\partial \mu_{k+1}}{\partial h}(h) \right|_{h=0} = \operatorname{ad}^*_{\xi_k} \operatorname{ad}^*_{\xi_k} \mu_k + \operatorname{ad}^*_{\dot{\xi}_k} \mu_k.$$

Comparing these derivatives with the Taylor expansion of the exact solution, we observe that

$$\mu_{k+1} = \mu(t_k + h) + \mathcal{O}(h^3).$$

Hence, the global error in μ_{k+1} is second order. Likewise for g_{k+1} we compute,

$$\frac{\partial g_{k+1}}{\partial h}(h)\bigg|_{h=0} = g_k \xi_k, \qquad \frac{\partial g_{k+1}}{\partial h}(h)\bigg|_{h=0} = g_k \dot{\xi}_k + g_k \xi_k^2.$$

From which it follows that

$$g_{k+1} = g(t_k + h) + \mathcal{O}(h^3).$$

■

4.8 Discrete Reduced HP Momentum Map Conservation

The manifold $\mathcal{I}_{hp}$ (cf. (3.6.4)) is a symplectic manifold with a discrete reduced symplectic form $\omega^d_{\mathcal{I}_{hp}}$ which will be defined shortly. Since a solution is uniquely determined by an initial $(g_0, \xi_0, \mu_0) \in \mathcal{I}_{hp}$, discrete reduced solution space can be identified with the finite-dimensional manifold $\mathcal{I}_{hp}$.

Consider once again the action of G on $G \times \mathfrak{g} \times \mathfrak{g}^*$, given by $\Phi^{G\times\mathfrak{g}\times\mathfrak{g}^*}$ (cf. (3.7.1)) and its infinitesimal generator $\psi^{G\times\mathfrak{g}\times\mathfrak{g}^*}$ (cf. (3.7.2)). For $x \in \mathfrak{g}$ the action of G on $G \times \mathfrak{g} \times \mathfrak{g}^*$ gives rise to two discrete reduced HP momentum maps J_k^+, J_k^- : $G \times \mathfrak{g} \times \mathfrak{g}^* \to \mathfrak{g}^*$,

$$J_k^+(g_k, \xi_k, \mu_k) \cdot x = h \left\langle \mu_k, d\tau^{-1}_{\xi_k} \left(\mathrm{Ad}_{g_k^{-1}} x \right) \right\rangle, \tag{4.8.1}$$

$$J_k^-(g_{k+1}, \xi_k, \mu_k) \cdot x = h \left\langle \mu_k, d\tau^{-1}_{-\xi_k} \left(\mathrm{Ad}_{g_{k+1}^{-1}} x \right) \right\rangle, \tag{4.8.2}$$

called the left- and right-reduced HP momentum maps respectively. Observe that they are in fact equal,

$$J_k^+ \cdot x = h \left\langle \mu_k, d\tau_{\xi_k}^{-1} \left(\mathrm{Ad}_{g_k^{-1} g_{k+1}} \mathrm{Ad}_{g_{k+1}^{-1}} x \right) \right\rangle = J_k^- \cdot x = J_k \cdot x.$$

The following theorem states that the unique momentum map introduced above, $J_k : G \times \mathfrak{g} \times \mathfrak{g}^* \to \mathfrak{g}^*$, is conserved under the discrete reduced HP flow.

Theorem 4.8.1. *The discrete reduced HP flow map preserves the unique reduced HP momentum map J_k.*

Proof. The action of G on the discrete curves $\mathcal{C}_d(G \times \mathfrak{g} \times \mathfrak{g}^*)$ is given by pointwise action

$$\Phi_s^{\mathcal{C}_d(G\times\mathfrak{g}\times\mathfrak{g}^*)}(\{g_k, \xi_k, \mu_k\}_{k=0}^N)(t_k) = \Phi_s^{G\times\mathfrak{g}\times\mathfrak{g}^*}(g_k, \xi_k, \mu_k),$$

and its infinitesimal generator is given by

$$\psi^{\mathcal{C}_d(G\times\mathfrak{g}\times\mathfrak{g}^*)}(\{g_k, \xi_k, \mu_k\}_{k=0}^N)(t_k) = \psi^{G\times\mathfrak{g}\times\mathfrak{g}^*}(g_k, \mu_k, \xi_k).$$

With these definitions it is straightforward to check the condition of infinitesimal symmetry,

$$\begin{aligned} & ds_d \cdot \psi^{\mathcal{C}_d(G\times\mathfrak{g}\times\mathfrak{g}^*)}(\{g_k, \xi_k, \mu_k\}) \\ &\quad = \sum_{k=0}^{N-1} \left[\left\langle \mu_k, d\tau_{h\xi_k}^{-1}(-\mathrm{Ad}_{g_k^{-1}} x) + d\tau_{-h\xi_k}^{-1}(\mathrm{Ad}_{g_{k+1}^{-1}} x) \right\rangle \right] h = 0. \end{aligned}$$

Consider the restriction of s_d to solution sequences: $\hat{s}_d : \mathcal{I}_{hp} \to \mathbb{R}$. By an application of summation by parts, the differential of $\hat{s}_d$ can be written as,

$$\begin{aligned} & d\hat{s}_d \cdot \psi^{G\times\mathfrak{g}\times\mathfrak{g}^*}(g_0, \xi_0, \mu_0) \\ &\quad = \sum_{k=1}^{N-1} \left[\left\langle \mu_k, d\tau_{h\xi_k}^{-1}(-\mathrm{Ad}_{g_k^{-1}} x) \right\rangle + \left\langle \mu_{k-1}, d\tau_{-h\xi_k}^{-1}(-\mathrm{Ad}_{g_k^{-1}} x) \right\rangle \right] h \\ &\quad\quad + \left\langle \mu_0, d\tau_{h\xi_0}^{-1}(-\mathrm{Ad}_{g_0^{-1}} x) \right\rangle h + \left\langle \mu_{N-1}, d\tau_{-h\xi_{N-1}}^{-1}(\mathrm{Ad}_{g_N^{-1}} x) \right\rangle h. \end{aligned}$$

And because of the restriction to solution sequences, $d\hat{s}_d$ can be simplified to

$$d\hat{s}_d \cdot \psi^{G\times\mathfrak{g}\times\mathfrak{g}^*}(g_0, \xi_0, \mu_0) = -J_0 \cdot x + J_N \cdot x = (-J_0 + (F_{hp}^N)^* J_0) \cdot x.$$

Moreover, due to infinitesimal symmetry, $J_0 = (F_{hp}^N)^* J_0$ which completes the proof.

■

The following examples evaluate (4.8.1) and (4.8.2) for various choices of F.

Examples

(a) Matrix Exponential. Suppose that τ is the exponential map. Then according to (4.6.4), one can write (4.8.1) and (4.8.2) as,

$$J_k^+(g_k, \xi_k, \mu_k) = h\left\langle \mathrm{Ad}^*_{g_k^{-1}}\left((\mathrm{dexp}^{-1}(h\xi_k))^*\mu_k\right), x\right\rangle,$$
$$J_k^-(g_{k+1}, \xi_k, \mu_k) \cdot x = h\left\langle \mathrm{Ad}^*_{g_{k+1}^{-1}}\left((\mathrm{dexp}^{-1}(-h\xi_k))^*\mu_k\right), x\right\rangle.$$

(b) Padé (1,1) Approximant. Suppose that τ is the Cayley map. Of course, we assume that the Lie group here is one in which the Cayley transform is a local diffeomorphism from the Lie algebra to that group. By (4.6.6) and (4.6.7), one can write (4.8.1) and (4.8.2) as,

$$J_k^+(g_k, \xi_k, \mu_k) = h\left\langle \mathrm{Ad}^*_{g_k^{-1}}\left((\mathrm{dcay}^{-1}(h\xi_k))^*\mu_k\right), x\right\rangle,$$
$$J_k^-(g_{k+1}, \xi_k, \mu_k) \cdot x = h\left\langle \mathrm{Ad}^*_{g_{k+1}^{-1}}\left((\mathrm{dcay}^{-1}(-h\xi_k))^*\mu_k\right), x\right\rangle.$$

(c) Padé (1,0) or (0,1) Approximant. Consider the case when $G = SO(n)$, where the skew projector ensures that the Padé (1,0) or (0,1) approximant to the exponential remains on the group. In this case using (4.6.9), (4.8.1) and (4.8.2) become,

$$J_k^+(g_k, \xi_k, \mu_k) = h\left\langle \mathrm{Ad}^*_{g_k^{-1}}\left((\mathrm{dskew}(h\xi_k))^*\mu_k\right), x\right\rangle,$$
$$J_k^-(g_{k+1}, \xi_k, \mu_k) \cdot x = h\left\langle \mathrm{Ad}^*_{g_{k+1}^{-1}}\left((\mathrm{dskew}(-h\xi_k))^*\mu_k\right), x\right\rangle.$$

4.9 Symplecticity of Discrete Reduced HP Flow Map

As before, by summation by parts, one can write the differential of the restricted reduced action sum $\hat{s}_d : \mathcal{I}_{hp} \to \mathbb{R}$ as,

$$\begin{aligned}
d\hat{s}_d \cdot (\delta g_0, \delta\xi_0, \delta\mu_0) &= \sum_{k=1}^{N-1} \left\langle \ell'(\xi_k) - \mu_k, \delta\xi_k \right\rangle + \left\langle \delta\mu_k, F(g_k^{-1} g_{k+1}) - \xi_k \right\rangle \\
&+ \left\langle \mu_k, d\tau^{-1}_{h\xi_k}(-\operatorname{Ad}_{g_k^{-1}} x) \right\rangle + \left\langle \mu_{k-1}, d\tau^{-1}_{-h\xi_k}(-\operatorname{Ad}_{g_k^{-1}} x) \right\rangle h \\
&+ \left\langle \mu_0, d\tau^{-1}_{h\xi_0}(-\operatorname{Ad}_{g_0^{-1}} x) \right\rangle h + \left\langle \mu_{N-1}, d\tau^{-1}_{-h\xi_{N-1}}(\operatorname{Ad}_{g_N^{-1}} x) \right\rangle h.
\end{aligned}$$

Only the boundary terms remain because of the restriction to solution sequences.

$$d\hat{s}_d \cdot (\delta g_0, \delta\xi_0, \delta\mu_0) = \left\langle \mu_0, d\tau^{-1}_{h\xi_0}(-\operatorname{Ad}_{g_0^{-1}} x) \right\rangle h + \left\langle \mu_{N-1}, d\tau^{-1}_{-h\xi_{N-1}}(\operatorname{Ad}_{g_N^{-1}} x) \right\rangle h.$$

These boundary terms define left and right one forms which are nearby the exact reduced HP one-form. To simplify the subsequent calculations the following one-forms, $\theta^+_{\mathcal{I}_{hp}}, \theta^-_{\mathcal{I}_{hp}} : T(\mathcal{I}_{hp}) \to \mathbb{R}$ are defined

$$\begin{aligned}
\theta^+_{\mathcal{I}_{hp}}(g_k, \xi_k, \mu_k) \cdot (\delta g_k, \delta\xi_k, \delta\mu_k) &= \left\langle \mu_k, d\tau^{-1}_{h\xi_k}(-g_k^{-1}\delta g_k) \right\rangle, \\
\theta^-_{\mathcal{I}_{hp}}(g_k, \xi_k, \mu_k) \cdot (\delta g_{k+1}, \delta\xi_{k+1}, \delta\mu_{k+1}) &= \left\langle \mu_k, d\tau^{-1}_{-h\xi_k}(g_{k+1}^{-1}\delta g_{k+1}) \right\rangle.
\end{aligned}$$

Although these one-forms are not equal, taking the second differential of one term of the reduced discrete action sum, it is apparent that

$$d\theta^+_{\mathcal{I}_{hp}}(g_k, \xi_k, \mu_k) = d\theta^-_{\mathcal{I}_{hp}}(g_k, \xi_k, \mu_k) = \omega^d_{\mathcal{I}_{hp}}(g_k, \xi_k, \mu_k).$$

That is, these one-forms define a unique discrete reduced symplectic two-form, $\omega^d_{\mathcal{I}_{hp}}$, on discrete reduced solution space.

In terms of these one-forms, the differential of $\hat{s}_d$ can be written as

$$d\hat{s}_d = (F^N_{hp})^* \theta^+_{\mathcal{I}_{hp}} - \theta^-_{\mathcal{I}_{hp}}.$$

Since $d^2\hat{s}_d = 0$ is zero, and since d and the pullback commute, observe that,

$$\begin{aligned} d^2\hat{s}_d &= d(F^N_{hp})^*\theta^+_{\mathcal{I}_{hp}}(g_0,\xi_0,\mu_0) - d\theta^-_{\mathcal{I}_{hp}}(g_0,\xi_0,\mu_0) \\ &= (F^N_{hp})^* d\theta^+_{\mathcal{I}_{hp}}(g_0,\xi_0,\mu_0) - d\theta^-_{\mathcal{I}_{hp}}(g_0,\xi_0,\mu_0) \end{aligned}$$

which implies that $(F^N_{hp})^*\omega^d_{\mathcal{I}_{hp}} = \omega^d_{\mathcal{I}_{hp}}$. And hence,

Theorem 4.9.1. *The discrete, reduced HP flow map preserves the discrete symplectic two-form* $\omega^d_{\mathcal{I}_{hp}}$.

Chapter 5

Free Rigid Body

In the absence of external forces and torques a rigid body preserves its total kinetic energy and is called *free*. The free rigid body is a left invariant Lagrangian system whose configuration space is SO(3) the set of 3×3 orthogonal matrices with determinant $+1$. Its tangent space is $T\,\mathrm{SO}(3)$ and phase space is the cotangent space $T^*\,\mathrm{SO}(3)$.

In what follows the following identification between an element of the Lie algebra of SO(3), $T_e\,\mathrm{SO}(3) = so(3)$, and $\mathbb{R}^3$ will be used. Recall that elements of $\mathfrak{so}(3)$ are skew-symmetric matrices with Lie bracket given by the matrix commutator. One can identify $\mathbb{R}^3$ with a skew-symmetric matrix via the hat map $\widehat{\cdot}: \mathbb{R}^3 \to so(3)$,

$$\widehat{\omega} = \begin{bmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{bmatrix}.$$

Let $g(t)$ be a curve in SO(3). With this identification of $\mathfrak{so}(3)$ to $\mathbb{R}^3$, the left-trivialization of a tangent vector $\dot{g}$ to this curve, given by $\xi = TL_{g^{-1}} \cdot \dot{g} \in \mathfrak{so}(3)$, can be written in terms of a body angular velocity vector $\mathbf{\Omega} \in \mathbb{R}^3$,

$$\xi = \widehat{\mathbf{\Omega}} \in so(3).$$

5.1 Lagrangian of Free Rigid Body

Let $\mathcal{B}$ denote a reference configuration of the body and $\rho : \mathbb{R}^3 \to \mathbb{R}$ denote the density of the body with respect to a body-fixed frame. Because the rigid body is free, the Lagrangian is given by its total kinetic energy which can be written as,

$$T = \frac{1}{2}\int_{\mathcal{B}} \rho(X)\|\hat{\boldsymbol{\Omega}} X\|^2 d^3X.$$

For a detailed derivation and exposition the reader is referred to [36, §15.1-15.3]. Since the body is rigid, this energy can be written in terms of a constant inertia matrix J,

$$\begin{aligned} T &= \frac{1}{2}\int_{\mathcal{B}} \rho(X)\boldsymbol{\Omega}^T \hat{X}^T \hat{X}\boldsymbol{\Omega} d^3X \\ &= \frac{1}{2}\boldsymbol{\Omega}^T \left(\int_{\mathcal{B}} \rho(X)\hat{X}^T\hat{X} d^3X\right)\boldsymbol{\Omega} \\ &= \frac{1}{2}\boldsymbol{\Omega}^T J\boldsymbol{\Omega}. \end{aligned}$$

This matrix is diagonal since it is assumed that the principal axis and body-fixed frame coincide. Alternatively, the total kinetic energy can be expressed in terms of a matrix J_d associated with a non-standard inertia tensor,

$$\begin{aligned} T &= \frac{1}{2}\int_{\mathcal{B}} \rho(X)\|\hat{\boldsymbol{\Omega}} X\|^2 d^3X \\ &= \frac{1}{2}\int_{\mathcal{B}} \rho(X)\,\mathrm{Trace}\left[\hat{\boldsymbol{\Omega}} X X^T \hat{\boldsymbol{\Omega}}^T\right] d^3X \\ &= \frac{1}{2}\,\mathrm{Trace}\left[\hat{\boldsymbol{\Omega}}\left(\int_{\mathcal{B}} \rho(X) X X^T d^3X\right)\hat{\boldsymbol{\Omega}}^T\right] \\ &= \frac{1}{2}\,\mathrm{Trace}\left[\hat{\boldsymbol{\Omega}} J_d \hat{\boldsymbol{\Omega}}^T\right]. \end{aligned}$$

The matrix J_d is related to J via,

$$\begin{aligned} J &= -\int_{\mathcal{B}} \rho(X)\hat{X}\hat{X}d^3X \\ &= \int_{\mathcal{B}} \rho(X)(-XX^T + X^TX\mathbf{Id})d^3X \\ &= -J_d + \mathrm{Trace}[J_d]\mathbf{Id}. \end{aligned}$$

Using the definition $\hat{\boldsymbol{\Omega}} = g^{-1}\dot{g}$ the following expression for the Lagrangian of the free rigid body, $L : T\,\mathrm{SO}(3) \to \mathbb{R}$, is obtained,

$$L(g,\dot{g}) = T = \frac{1}{2}\,\mathrm{Trace}\left[(g^{-1}\dot{g})J_d(g^{-1}\dot{g})^T\right].$$

Observe that L is left invariant on SO(3) since for any $B \in \mathrm{SO}(3)$,

$$L(Bg, B\dot{g}) = \frac{1}{2}\,\mathrm{Trace}\left[(g^{-1}B^{-1}B\dot{g})J_d(g^{-1}B^{-1}B\dot{g})^T\right] = L(g,\dot{g}).$$

The reduced Lagrangian is given by restricting L to $\mathfrak{so}(3)$,

$$\ell(\xi) = L(e,\xi) = \frac{1}{2}\,\mathrm{Trace}\left[\xi^T J_d \xi\right] = \frac{1}{2}\left\langle\left\langle \xi, \xi \right\rangle\right\rangle.$$

Adjoint action of SO(3) and $\mathfrak{so}(3)$. Using the identification to $\mathbb{R}^3$, the adjoint action of SO(3) on $\mathfrak{so}(3)$ is left multiplication by g, i.e., for $\hat{\mathbf{x}}, \hat{\mathbf{y}} \in \mathfrak{so}(3)$,

$$\hat{\mathbf{y}} = \mathrm{Ad}_g\,\hat{\mathbf{x}} = g\hat{\mathbf{x}}g^{-1} = \widehat{g\mathbf{x}} \implies \mathbf{y} = g\mathbf{x}.$$

Similarly, the coadjoint action is left multiplication by g^* since, for $\hat{\mathbf{x}}, \hat{\mathbf{y}} \in \mathfrak{so}(3)^*$,

$$\hat{\mathbf{y}} = \mathrm{Ad}_g^*\,\hat{\mathbf{x}} = g^*\hat{\mathbf{x}}g = \widehat{g^*\mathbf{x}} \implies \mathbf{y} = g^*\mathbf{x}.$$

The adjoint action of $\mathfrak{so}(3)$ on itself is determined from the commutator bracket. For $x, y \in \mathbb{R}^3$, the action takes the form,

$$\mathrm{ad}_{\widehat{x}}\,\widehat{y} = [\widehat{x}, \widehat{y}] = \widehat{\widehat{x}y},$$

which can be written more simply using the identification to $\mathbb{R}^3$ as,

$$\mathrm{ad}_x\, y = \widehat{x} y.$$

Likewise, the coadjoint action of $\mathfrak{se}(3)$ on its dual is given by,

$$\mathrm{ad}^*_{\widehat{x}}\, \widehat{y} = [\widehat{x}^*, \widehat{y}] = \widehat{\widehat{y}x},$$

which has the expression,

$$\mathrm{ad}^*_x\, y = \widehat{y} x.$$

5.2 Euler's Equations on $\mathfrak{so}(3)$

The dynamics of a free rigid body is described by Euler's equations. These are the reduced HP equations on $\mathrm{SO}(3) \times \mathfrak{so}(3) \times \mathfrak{so}(3)^*$ for this Lagrangian system. These equations are written down explicitly here. Let $\mathbf{\Pi} \in \mathbb{R}^3$ be the body angular momentum associated with μ via the hat map $\mu = \widehat{\mathbf{\Pi}} \in \mathfrak{so}(3)^*$. Then (3.6.1) take the form,

$$\dot{\mathbf{\Pi}} = \mathrm{ad}^*_{\mathbf{\Omega}}\, \mathbf{\Pi} = \widehat{\mathbf{\Pi}} \mathbf{\Omega}.$$

The operator form of the reduced Legendre transform (3.6.2) is given by,

$$\left\langle \ell'(\xi) - \mu, \delta\xi \right\rangle = 0$$

for arbitrary variations $\delta\xi \in \mathfrak{so}(3)$. Using basic properties of the trace this can be written as,

$$\begin{aligned}\left\langle \ell'(\xi) - \mu, \delta\xi \right\rangle &= \frac{1}{2}\,\mathrm{Trace}\left[(J_d\xi - \mu)^* \delta\xi\right] \\ &= \frac{1}{4}\,\mathrm{Trace}\left[\delta\xi^* (J_d\xi + \xi J_d - \mu)\right].\end{aligned}$$

Since this pairing is non-degenerate and $\delta\xi$ is arbitrary,

$$\ell'(\xi) = \xi J_d + J_d \xi = \mu.$$

One can write the above in terms of $\mathbf{\Pi}$ and $\mathbf{\Omega}$ using the identity,

$$\widehat{J\mathbf{\Omega}} = \hat{\mathbf{\Omega}} J_d + J_d \hat{\mathbf{\Omega}}.$$

This identity can be directly verified as follows. Let $(\mathbf{e}_i, \mathbf{e}_j, \mathbf{e}_k)$ be an orthonormal frame fixed to the body. Then, on the one hand using the scalar triple product rule,

$$\begin{aligned}\mathbf{e}_i^T \widehat{J\mathbf{\Omega}} \mathbf{e}_j &= -(J\mathbf{\Omega})^T \hat{\mathbf{e}}_i \mathbf{e}_j \\ &= -(J\mathbf{\Omega})^T \mathbf{e}_k = -J_k \mathbf{\Omega}^T \mathbf{e}_k.\end{aligned}$$

On the other hand,

$$\begin{aligned}\mathbf{e}_i^T \left(\hat{\mathbf{\Omega}} J_d + J_d \hat{\mathbf{\Omega}}\right) \mathbf{e}_j &= \mathbf{e}_i^T \left(\mathrm{Trace}[J] \hat{\mathbf{\Omega}} - \hat{\mathbf{\Omega}} J - J \hat{\mathbf{\Omega}}\right) \mathbf{e}_j \\ &= -\mathrm{Trace}[J] \mathbf{\Omega}^T \hat{\mathbf{e}}_i{}^T \mathbf{e}_j - J_j \mathbf{\Omega}^T \hat{\mathbf{e}}_j \mathbf{e}_i - J_i \mathbf{\Omega}^T \hat{\mathbf{e}}_j \mathbf{e}_i \\ &= -(J_i + J_j + J_k) \mathbf{\Omega}^T (\mathbf{e}_k) + (J_j + J_i) \mathbf{\Omega}^T (\mathbf{e}_k) \\ &= -J_k \mathbf{\Omega}^T \mathbf{e}_k.\end{aligned}$$

Thus,

$$\widehat{J\mathbf{\Omega}} = \hat{\mathbf{\Omega}} J_d + J_d \hat{\mathbf{\Omega}} = \xi J_d + J_d \xi = \mu = \widehat{\mathbf{\Pi}}.$$

The reduced HP equations (3.6.1)-(3.6.3) for the free rigid body follow,

$$\dot{g} = g \widehat{\mathbf{\Omega}}, \tag{5.2.1}$$

$$\mathbf{\Pi} = J \mathbf{\Omega}, \tag{5.2.2}$$

$$\dot{\mathbf{\Pi}} = \widehat{\mathbf{\Pi}} \mathbf{\Omega}. \tag{5.2.3}$$

Observe that the last two equations are decoupled from the Lie group. To reconstruct the solution on SO(3) from the solution to the last two equations, the initial value problem $\dot{g} = g\widehat{\mathbf{\Omega}}$ is solved for $g \in \mathrm{SO}(3)$.

Conservation of spatial angular momentum. Let $\boldsymbol{\pi} \in \mathbb{R}^3$ be the vector associated with the spatial angular momentum $\mu_s \in \mathfrak{so}(3)^*$ via the hat map, i.e., $\widehat{\boldsymbol{\pi}} = \mu_s$. From (3.7.3) for $x \in \mathbb{R}^3$, the preserved momentum map is,

$$\begin{aligned} J(g, \xi, \mu) \cdot \hat{x} &= \left\langle \mathrm{Ad}^*_{g^{-1}} \mu, \hat{x} \right\rangle \\ &= \frac{1}{2} \operatorname{Trace}\left[\mu_s^* \hat{x}\right] = -\frac{1}{2} \operatorname{Trace}\left[\hat{x} \hat{\boldsymbol{\pi}}\right]. \end{aligned}$$

Simplifying the above expression gives,

$$\begin{aligned} J(g, \xi, \mu) \cdot \hat{x} &= \frac{1}{2} \operatorname{Trace}\left[(x^T \boldsymbol{\pi}) e - \boldsymbol{\pi} x^T\right] \\ &= \frac{3}{2} x^T \boldsymbol{\pi} - \frac{1}{2} x^T \boldsymbol{\pi} = x^T \boldsymbol{\pi}. \end{aligned}$$

And since x is arbitrary and the pairing non-degenerate, $\boldsymbol{\pi}$ is the conserved momentum map.

The spatial and body angular momenta are related via the coadjoint action on $\mathfrak{so}(3)^*$,

$$\mu_s = \hat{\boldsymbol{\pi}} = \mathrm{Ad}^*_{g^{-1}} \hat{\mathbf{\Pi}} = \mathrm{Ad}^*_{g^{-1}} \mu.$$

And with the identification to $\mathbb{R}^3$ this is simply $\boldsymbol{\pi} = g\mathbf{\Pi}$.

5.3 TLN and FLV for Euler's Equations

In this section the TLN and FLV method will be tested on the free rigid body and compared for various time-step sizes. In specializing these methods to SO(3), the identification of a 3-vector to an element of $\mathfrak{so}(3)$ is used. With this identification the TLN algorithm for free rigid bodies will be derived in detail. Carrying this procedure out for MLN and FLV is very similar and therefore omitted.

Evaluating TLN for the reduced Lagrangian of the rigid body gives,

$$\mu_{k+1} = \mu_k + \frac{h}{2}\left(\operatorname{ad}^*_{\xi_k}\mu_k + \operatorname{ad}^*_{\xi_{k+1}}\mu_{k+1}\right)$$

since $\mu_k = \ell'(\xi_k)$. Using the identification to $\mathbb{R}^3$ given by

$$\xi_k = \widehat{\boldsymbol{\Omega}}_k, \qquad \mu_k = \widehat{\boldsymbol{\Pi}}_k$$

the difference scheme can be written as,

$$\boldsymbol{\Pi}_{k+1} = \boldsymbol{\Pi}_k + \frac{h}{2}\left(\operatorname{ad}^*_{\boldsymbol{\Omega}_k}\boldsymbol{\Pi}_k + \operatorname{ad}^*_{\boldsymbol{\Omega}_{k+1}}\boldsymbol{\Pi}_{k+1}\right),$$

or in terms of the cross product in $\mathbb{R}^3$ as,

$$\boldsymbol{\Pi}_{k+1} = J\boldsymbol{\Omega}_{k+1} = \boldsymbol{\Pi}_k - \frac{h}{2}\left(\widehat{\boldsymbol{\Omega}_k}\boldsymbol{\Pi}_k + \widehat{\boldsymbol{\Omega}_{k+1}}\boldsymbol{\Pi}_{k+1}\right).$$

This difference scheme together with the reconstruction equation

$$g_{k+1} = g_k \operatorname{cay}(h\boldsymbol{\Omega}_k)$$

defines the TLN on SO(3). Table 5.1 lists the defining DEP schemes for each method.

Table 5.1: **LN and FLV for Euler's Equations**

Method	Defining Difference Equation
TLN	$\boldsymbol{\Omega}_{k+1} = \boldsymbol{\Omega}_k + h/2J^{-1}\left(\widehat{J\boldsymbol{\Omega}_k} + \widehat{J\boldsymbol{\Omega}_{k+1}}\right)$
MLN	$\boldsymbol{\Omega}_{k+1} = \boldsymbol{\Omega}_k + hJ^{-1}\left(\widehat{J\boldsymbol{\Omega}_{k+1/2}}\boldsymbol{\Omega}_{k+1/2}\right)$
FLV	$\boldsymbol{\Omega}_{k+1} = \boldsymbol{\Omega}_{k-1} + hJ^{-1}\left(\widehat{J\boldsymbol{\Omega}_{k+1/2}} + \widehat{J\boldsymbol{\Omega}_{k-1/2}}\right)\boldsymbol{\Omega}_k$

5.4 HPVI for Euler's Equations

Let $x \in \mathbb{R}^3$. Using cross product identities, one can write any real analytic function $\tau : \mathfrak{so}(3) \to \mathrm{SO}(3)$ as,

$$\tau(x) = e + c_1(\theta)\hat{x} + c_2(\theta)\hat{x}^2, \quad \theta = \sqrt{x^T x} = \|x\|. \tag{5.4.1}$$

See e.g. [19]. Assuming τ is a local diffeomorphism, then in terms of τ a HPVI for Euler's equations can be written as:

$$g_{k+1} = g_k \tau(h\mathbf{\Omega}_k) \quad \text{(reconstruction equation)}, \tag{5.4.2}$$

$$\mathbf{\Pi}_k = J\mathbf{\Omega}_k \quad \text{(reduced Legendre transform)}, \tag{5.4.3}$$

$$(d\tau^{-1}_{h\mathbf{\Omega}_k})^* \mathbf{\Pi}_k = (d\tau^{-1}_{-h\mathbf{\Omega}_{k-1}})^* \mathbf{\Pi}_{k-1} \quad \text{(discrete LP equation)}. \tag{5.4.4}$$

In addition to being a local diffeomorphism, it is assumed that τ is a second-order approximation to the exponential map. In the context of SO(3), this assumption implies that

$$c_1 = 1 + O(\theta^2), \quad c_2 = 1/2 + O(\theta).$$

In what follows a general expression for the right trivialized tangent of τ in the context of SO(3) is derived.

Lemma 5.4.1. *If $\tau(x) \in \mathrm{SO}(3)$ is given by (5.4.1) then*

$$2c_2 - c_2^2\theta^2 = c_1^2.$$

Proof. If $\tau(x) \in \mathrm{SO}(3)$, then $\tau(x)\tau(x)^{\mathrm{T}} = \tau(x)\tau(-x) = e$ and $\det(\tau(x)) = 1$. Expanding the former using (5.4.1) gives:

$$\begin{aligned}\tau(x)\tau(-x) &= (e + c_1\hat{x} + c_2\hat{x}^2)(e - c_1\hat{x} + c_2\hat{x}^2) \\ &= e - c_1^2\hat{x}^2 + 2c_2\hat{x}^2 + c_2^2\hat{x}^4.\end{aligned}$$

However, since $\hat{x}^3 = -\theta^2\hat{x}$ and $\hat{x}^4 = -\theta^2\hat{x}^2$,

$$\tau(x)\tau(-x) = e + (-c_1^2 + 2c_2 - c_2^2\theta^2)\hat{x}^2$$

Since x is an arbitrary 3-vector, the orthogonality condition is satisfied if and only if c_1 and c_2 satisfy: $2c_2 - c_2^2\theta^2 = c_1^2$. Moreover

$$\det(\tau(x)) = c_1^2\theta^2 + (-1 + c_2\theta^2)^2 = \theta^2(c_1^2 - 2c_2 + c_2^2\theta^2) + 1.$$

For arbitrary $\theta \neq 0$, $\det(\tau(x)) = 1$ if and only if $2c_2 - c_2^2\theta^2 = c_1^2$. ■

Lemma 5.4.2. *If $\tau(x)$ is given by (5.4.1) and $\tau(x) \in \mathrm{SO}(3)$ then its right-trivialized tangent is given by*

$$d\tau_x(\delta) = c_1\delta + c_2\hat{x}\delta + c_3 x^T\delta x,$$

where

$$c_3 = \frac{c_2' + c_2^2\theta}{c_1\theta}.$$

Proof. This formula can be derived directly from the derivative of τ and using the definition of the right trivialized tangent. The derivative of τ is given by

$$\begin{aligned}\mathrm{D}\,\tau(x)\cdot\delta &= \widehat{d\tau_x(\delta)}\tau(x) \\ &= (c_1'\hat{x} + c_2'\hat{x}^2)x^T\delta/\theta + c_1\hat{\delta} + c_2(\hat{x}\hat{\delta} + \hat{\delta}\hat{x})\end{aligned}$$

Solving for $\widehat{d\tau_x(\delta)}$ gives,

$$\begin{aligned}\widehat{d\tau_x(\delta)} &= (c_1'\hat{x} + c_2'\hat{x}^2)x^{\mathrm{T}}\delta/\theta + c_1\hat{\delta} + c_2(\hat{x}\hat{\delta} + \hat{\delta}\hat{x}) \\ &\quad - (c_1c_1'\hat{x}^2 + c_1c_2'\hat{x}^3)x^{\mathrm{T}}\delta/\theta - c_1^2\hat{\delta}\hat{x} - c_2c_1(\hat{x}\hat{\delta}\hat{x} + \hat{\delta}\hat{x}^2) \\ &\quad + (c_2c_1'\hat{x}^3 + c_2c_2'\hat{x}^4)x^{\mathrm{T}}\delta/\theta + c_1c_2\hat{\delta}\hat{x}^2 + c_2^2(\hat{x}\hat{\delta}\hat{x}^2 + \hat{\delta}\hat{x}^3).\end{aligned}$$

Simplifying the above using the identities $\hat{x}^3 = -\theta^2 \hat{x}$ and $\hat{x}^4 = -\theta^2 \hat{x}^2$ yields

$$\begin{aligned}\widehat{d\tau_x(\delta)} = c_1\hat{\delta} + c_2(\hat{x}\hat{\delta} + \hat{\delta}\hat{x}) - (\theta^2 c_2^2 + c_1^2)\hat{\delta}\hat{x} \\ + x^T\delta(\theta c_1 c_2' + c_2 c_1 - \theta c_2 c_1' + c_1'/\theta)\hat{x} \\ + x^T\delta(c_2'/\theta - c_1 c_1'/\theta - \theta c_2 c_2' - c_2^2)\hat{x}^2.\end{aligned}$$

This can be written in the more revealing form:

$$\begin{aligned}\widehat{d\tau_x(\delta)} = c_1\hat{\delta} + c_2(\hat{x}\hat{\delta} + \hat{\delta}\hat{x}) - (\theta^2 c_2^2 + c_1^2)\hat{\delta}\hat{x} \\ + x^T\delta(\theta c_1 c_2' + c_2 c_1 - \theta c_2 c_1' + c_1'/\theta)\hat{x} \\ + \frac{1}{2\theta}\left(\mathrm{D}\left[2c_2 - c_2^2\theta^2 - c_1^2\right]\cdot\delta\right)\hat{x}^2.\end{aligned}$$

Using lemma (5.4.1) and $(\hat{x}\hat{\delta} - \hat{\delta}\hat{x}) = \widehat{\hat{x}\delta}$ gives the desired result:

$$\begin{aligned}\widehat{d\tau_x(\delta)} =& c_1\hat{\delta} + c_2(\hat{x}\hat{\delta} - \hat{\delta}\hat{x}) \\ & + x^T\delta/\theta(\theta c_1 c_2 + c_1' + \theta^2(c_1 c_2' - c_1' c_2))\hat{x} \\ =& c_1\hat{\delta} + c_2\widehat{\hat{x}\delta} + \frac{c_2' + c_2^2\theta}{c_1\theta}x^T\delta\hat{x}.\end{aligned}$$

■

Lemma 5.4.3. *If $\tau(x)$ is given by (5.4.1) and $\tau(x) \in \mathrm{SO}(3)$ then the right trivialized tangent of τ^{-1} is given by*

$$d\tau_x^{-1}(\delta) = \frac{c_1}{2c_2}\delta - \frac{1}{2}\hat{x}\delta + \alpha_3 x^T\delta x,$$

where α_3 satisfies:

$$\frac{c_2'}{c_2\theta} + 2\alpha_3\frac{2c_2 + c_2'\theta}{c_1} = 0.$$

Proof. Let $d\tau_x^{-1}(\delta) = \alpha_1\delta + \alpha_2\hat{x}\delta + \alpha_3 x^T\delta x$. Then by definition of the right trivialized tangent of τ and τ^{-1},

$$d\tau_x^{-1}(d\tau_x(\delta)) = \delta.$$

Expanding the left-hand side using lemma 5.4.2 yields,

$$\begin{aligned}
d\tau_x^{-1}(d\tau_x(\delta)) =& \alpha_1 c_1 \delta + \alpha_1 c_2 \hat{x}\delta + \alpha_2 c_1 \hat{x}\delta + \alpha_2 c_2 \hat{x}^2 \delta + x^T \delta(\alpha_3 c_1 + \alpha_3 c_3 \theta^2 + \alpha_1 c_3) x \\
=& (\alpha_1 c_1 - \theta^2 \alpha_2 c_2)\delta + (\alpha_1 c_2 + \alpha_2 c_1)\hat{x}\delta \\
& + x^T \delta(\alpha_2 c_2 + \alpha_3 c_1 + \alpha_3 c_3 \theta^2 + \alpha_1 c_3) x \\
=& \delta
\end{aligned}$$

Equating coefficients of δ, $\hat{x}\delta$ and $x^T \delta x$ gives,

$$\begin{aligned}
\alpha_1 c_1 - \theta^2 \alpha_2 c_2 &= 1, \\
\alpha_1 c_2 + \alpha_2 c_1 &= 0, \\
\alpha_2 c_2 + \alpha_3 c_1 + \alpha_3 c_3 \theta^2 + \alpha_1 c_3 &= 0.
\end{aligned}$$

The first two algebraic equations can be written in matrix-form,

$$\begin{bmatrix} c_1 & -\theta^2 c_2 \\ c_2 & c_1 \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

Using lemma 5.4.1 notice that the determinant of the matrix is $c_1^2 + \theta^2 c_2^2 = 2c_2$, and

$$c_1^2 + \theta^2 c_2^2 \geq 0.$$

For $\theta_0 \neq 0$, equality happens only when $c_1(\theta_0) = c_2(\theta_0) = 0$. However, if this is true then τ is no longer a local diffeomorphism. And if $c_2 = 0$ for all θ, then by the same lemma, $c_1 = 0$ for all θ and τ is not a local diffeomorphism. Assuming that $c_2 > 0$, one can solve this system to obtain $\alpha_1 = c_1/(2c_2)$ and $\alpha_2 = -1/2$. Substituting these solutions into the third equation and simplifying yields the equation α_3 satisfies. ∎

5.5 TLN as an HPVI

The trapezoidal Lie-Newmark (TLN) scheme is given by:

$$g_{k+1} = g_k \operatorname{cay}(h\boldsymbol{\Omega}_k), \tag{5.5.1}$$

$$\boldsymbol{\Pi}_k = J\boldsymbol{\Omega}_k, \tag{5.5.2}$$

$$\boldsymbol{\Pi}_k - \frac{h}{2}\widehat{\boldsymbol{\Pi}_k}\boldsymbol{\Omega}_k = \boldsymbol{\Pi}_{k-1} + \frac{h}{2}\widehat{\boldsymbol{\Pi}_{k-1}}\boldsymbol{\Omega}_{k-1}. \tag{5.5.3}$$

If TLN is derived from the reduced HP principle on SO(3) then,

$$d\tau_x^{-1}(\delta) = \delta - \frac{1}{2}\hat{x}\delta.$$

Can one obtain a τ with a $d\tau_x^{-1}$ of this form? Using the lemmas it is straightforward to show if you assume a right trivialized tangent of τ^{-1} of the desired form (5.5.4), then the coefficients are uniquely determined, i.e.,

$$d\tau_x^{-1}(\delta) = \sqrt{1 - \frac{\theta}{4}}\delta - \frac{1}{2}\hat{x}\delta.$$

Thus, TLN is not an HPVI in this sense.

Theorem 5.5.1. *Consider a real analytic function $\tau : \mathfrak{so}(3) \to \mathrm{SO}(3)$ that is a local diffeomorphism. Suppose the right trivialized tangent of τ^{-1} takes the form*

$$d\tau_x^{-1}(\delta) = \alpha_1\delta + \alpha_2\hat{x}\delta. \tag{5.5.4}$$

Then c_2 = constant, $c_1 = \sqrt{2c_2 - c_2^2\theta}$, $\alpha_1 = c_1/(2c_2)$, and $\alpha_2 = -1/2$. If one further requires that τ is a second order approximation to the exact exponential map, then $c_2 = 1/2$, $c_1 = \sqrt{1 - \theta/4}$ and $\alpha_1 = \sqrt{1 - \theta/4}$.

Summary of HPVIs The coefficients in τ and $d\tau^{-1}$ for several HPVIs tested are written down explicitly in what follows.

- Exponential-based scheme (EXP):

$$c_1 = \frac{\sin(\theta)}{\theta}, \quad c_2 = \frac{1}{2}\frac{\sin^2(\theta/2)}{(\theta/2)^2}, \quad \alpha_1 = \frac{1}{2}\theta\cot(\theta/2), \quad \alpha_3 = \frac{2-\theta\cot(\theta/2)}{2\theta^2}.$$

- Cayley-based scheme (CAY):

$$c_1 = \frac{4}{4+\theta^2}, \quad c_2 = \frac{2}{4+\theta^2}, \quad \alpha_1 = 1, \quad \alpha_3 = \frac{1}{4}.$$

- NEW-scheme (NEW):

$$c_1 = \sqrt{1-\theta^2/4}, \quad c_2 = 1/2, \quad \alpha_1 = \sqrt{1-\theta^2/4}, \quad \alpha_3 = 0.$$

- Skew-scheme (SKEW):

$$c_1 = 1, \quad c_2 = \frac{1-\sqrt{1-\theta^2}}{\theta^2}, \quad \alpha_1 = \frac{1}{2}(1+\sqrt{1-\theta^2}), \quad \alpha_3 = -\frac{1}{2+2\sqrt{1-\theta^2}}.$$

5.6 Coadjoint and Energy-Preserving Methods for Euler's Equations

The explicit coadjoint-preserving Simo & Wong method (SW) specialized to the free rigid body takes the following form,

$$\begin{aligned} g_{k+1} &= g_k \exp(\mathbf{\Theta}_k) \\ \mathbf{\Pi}_k &= J\mathbf{\Omega}_k \\ \mathbf{\Pi}_{k+1} &= \exp(-\mathbf{\Theta}_k)\mathbf{\Pi}_k \end{aligned}$$

where $\mathbf{\Theta}_k$ is determined by:

$$\mathbf{\Theta}_k = h\mathbf{\Omega}_k + \frac{h^2}{2}\dot{\mathbf{\Omega}}_k.$$

To project onto the energy level-set, the following intermediate variable $\widetilde{\mathbf{\Theta}}_k$

and algebraic energy constraint are introduced,

$$\mathcal{H}(\mathbf{\Theta}_k) = \mathbf{\Pi}_k^T \exp(\mathbf{\Theta}_k) J^{-1} \exp(-\mathbf{\Theta}_k)\mathbf{\Pi}_k/2,$$
$$\widetilde{\mathbf{\Theta}}_k = h\mathbf{\Omega}_k + \frac{h^2}{2}\dot{\mathbf{\Omega}}_k.$$

The energy and coadjoint-preserving Simo & Wong method (SW⊥) is given by:

$$\mathbf{\Theta}_k = \widetilde{\mathbf{\Theta}}_k + \lambda \mathcal{H}_\Theta(\widetilde{\mathbf{\Theta}}_k), \quad \mathcal{H}(\mathbf{\Theta}_k) = \mathcal{H}_0$$

While the KR method:

$$\mathbf{\Theta}_k = \lambda \widetilde{\mathbf{\Theta}}_k, \quad \mathcal{H}(\mathbf{\Theta}_k) = \mathcal{H}_0.$$

This construction of Krysl's method is the same as that in Krysl's paper modulo semantic differences [23]. These schemes extend the explicit momentum-preserving schemes due to Simo & Wong by endowing the scheme with energy conservation properties [46]. Notice that the KR scheme determines λ by enforcing energy conservation which is satisfied if λ is a root of $f : \mathbb{R} \to \mathbb{R}$ defined as,

$$f(\lambda) = \mathbf{\Pi}_k^T \exp(\lambda \widetilde{\mathbf{\Theta}}_k) J^{-1} \exp(-\lambda \widetilde{\mathbf{\Theta}}_k)\mathbf{\Pi}_k - \mathbf{\Pi}_k^T \mathbb{I}^{-1} \mathbf{\Pi}_k. \tag{5.6.1}$$

This nonlinear scalar equation, $f(\lambda) = 0$, has a solution since it is trivially satisfied at $\lambda = 0$ and periodic in λ. Any root-finding method (e.g. Newton's method) can be used to solve for λ. The initial condition for this root finder is chosen to be $\lambda \approx 1$. The method is considered semi-explicit since it is only implicit in the scalar unknown λ at every timestep [23]. These coadjoint and energy-preserving algorithms are summarized in the following table.

For a more detailed discussion of SW, SW⊥, and KR, the reader is referred to [6].

Table 5.2: **Energy-Momentum Methods for Euler's Equations**

Method	Definition of Relative Rotation Vector
SW	$\mathbf{\Theta}_k = h\mathbf{\Omega}_k + h^2/2\dot{\mathbf{\Omega}}_k$
SW⊥	$\mathbf{\Theta}_k = \widetilde{\mathbf{\Theta}}_k + \lambda\mathcal{H}_\Theta(\widetilde{\mathbf{\Theta}}_k), \quad \mathcal{H}(\mathbf{\Theta}_k) = \mathcal{H}_0$
KR	$\mathbf{\Theta}_k = \lambda\widetilde{\mathbf{\Theta}}_k, \quad \mathcal{H}(\mathbf{\Theta}_k) = \mathcal{H}_0$

5.7 Simulation Results for Euler's Equations.

Here the structure-preserving Lie group methods are applied to free rigid body dynamics. A quantitative comparison of the performance of EXP, NEW, SKE, CAY, TLN, FLV, KR, and SWP is provided in Fig. 5.7.1. It shows CPU times for all methods tested as a function of precision. The FLV and SWa methods are clearly the top two performers overall. The figure also reveals that although the HPVIs tested are second-order accurate, the error constant at $o(h^2)$ is larger in comparison to the other methods.

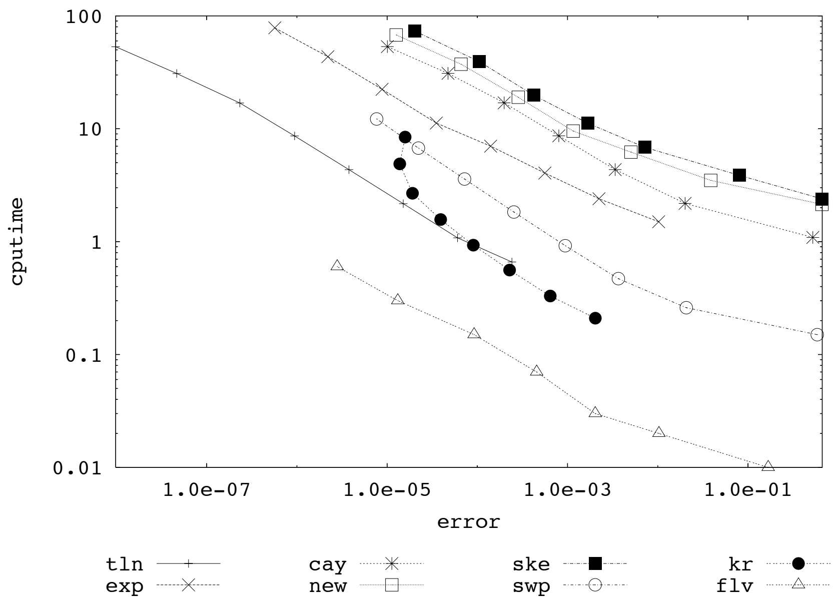


Figure 5.7.1: **Work precision diagram for Euler's equations.** This diagram shows CPU times in seconds vs. precision for the methods tested on the free rigid body. The top performer is FLV followed by TLN and KR.

Chapter 6

Underwater Vehicle

Consider a rigid body submerged in an infinitely large volume of incompressible, irrotational and invisicid fluid that is at rest at infinity. In the absence of external forces, and under the approximations that the fluid is incompressible, irrotational, and inviscid, and the body is neutrally buoyant, the configuration manifold of a underwater vehicle is $SE(3)$ and the dynamics is EP. For a recent application of this system to the study of fish locomotion the reader is referred to [33]. For an application of a related model of articulated rigid bodies to the study of more complex fish locomotion the reader is referred to [21].

Let $g(t)$ be a curve in $SE(3)$. An element of $SE(3)$ can be identified with an element of $SL(4;\mathbb{R})$ through the map

$$g = \begin{bmatrix} B & \mathbf{x} \\ \mathbf{0} & 1 \end{bmatrix}; \quad B \in \mathrm{SO}(3); \quad \mathbf{x} \in \mathbb{R}^3.$$

The group action is simply matrix multiplication. The inverse is given by

$$g^{-1} = \begin{bmatrix} B^T & -B^T\mathbf{x} \\ \mathbf{0} & 1 \end{bmatrix}.$$

The left-trivialization of a tangent vector $\dot{g}$ to the curve $g(t)$ is given by

$$\xi = \begin{bmatrix} \widehat{\mathbf{\Omega}} & \mathbf{v} \\ \mathbf{0} & 0 \end{bmatrix} \in \mathfrak{se}(3); \quad \widehat{\mathbf{\Omega}} \in so(3); \quad \mathbf{v} \in \mathbb{R}^3.$$

where $\mathbf{v} = B^T \dot{\mathbf{x}}$ and $\widehat{\mathbf{\Omega}} = B^T \dot{B}$. Thus, one can identify $se(3)$ with $\mathbb{R}^3 \times \mathbb{R}^3$.

6.1 Lagrangian of Underwater Vehicle

The Lagrangian of a rigid body in ideal fluid is left invariant and simply the sum of the rotational and translational kinetic energy of the body and the kinetic energy of the surrounding fluid, i.e.,

$$L = T_{\mathcal{F}} + T_{\mathcal{B}}.$$

Let $\mathcal{F} \subset \mathbb{R}^3$ denote the region occupied by the fluid, ρ_F the density of the fluid, and $\boldsymbol{u}$ the spatial velocity field of the fluid. The kinetic energy of the fluid is then given by,

$$T_{\mathcal{F}} = \frac{1}{2}\rho_F \int_{\mathcal{F}} \|\boldsymbol{u}(x)\|^2 d^3x.$$

One can write $T_{\mathcal{F}}$ as a function of only the variables associated with the solid body by following the classical procedure of Kirchhoff [24]. Thus, up to added mass and inertia terms, the fluid is decoupled from the submerged body. The procedure to do this is outlined here.

Since the flow is irrotational (curl free) the velocity $\mathbf{u}$ of the ambient fluid can be expressed as the gradient of some potential field, i.e.,

$$\mathbf{u} = -\nabla\phi = \left(-\frac{\partial\phi}{\partial x}, -\frac{\partial\phi}{\partial y}, -\frac{\partial\phi}{\partial z}\right).$$

Since the fluid is incompressible the continuity equation implies that $\nabla \cdot \mathbf{u} = 0$ or that,

$$\nabla \cdot \mathbf{u} = \nabla^2\phi = 0$$

Let $\mathbf{n}$ be the normal vector to the surface of the body. Let v_n denote the velocity of the body projected in the direction of $\mathbf{n}$. The condition that the fluid does not penetrate the solid body is formulated as

$$\mathbf{u} \cdot \mathbf{n} = -\nabla\phi \cdot \mathbf{n} = v_n.$$

The condition that the fluid is at rest at infinity is formulated as

$$\frac{\partial \phi}{\partial x} = 0, \quad \frac{\partial \phi}{\partial y} = 0, \quad \frac{\partial \phi}{\partial z} = 0.$$

Let $\boldsymbol{v} = (v_1, v_2, v_3) \in \mathbb{R}^3$ and $\boldsymbol{\Omega} = (\Omega_1, \Omega_2, \Omega_3) \in \mathbb{R}^3$ be the components of the translational and rotational velocity of the body in a body-fixed frame. Under the assumptions above, Kirchhoff showed that the potential can be written in terms of $\boldsymbol{v}$ and $\boldsymbol{\Omega}$,

$$\phi = v_1\phi_1 + v_2\phi_2 + v_3\phi_3 + \Omega_1\chi_1 + \Omega_2\chi_2 + \Omega_3\chi_3.$$

Since the fluid motion is the gradient of a potential field and divergence free, the kinetic energy of the fluid can be written as,

$$\begin{aligned} T_{\mathcal{F}} &= \frac{1}{2}\rho_F \int_{\mathcal{F}} \|\boldsymbol{u}(x)\|^2 d^3x \\ &= \rho_F \int_{\mathcal{F}} \left(\frac{\partial \phi}{\partial x}^2 + \frac{\partial \phi}{\partial y}^2 + \frac{\partial \phi}{\partial z}^2 \right) d^3x \\ &= \rho_F \int_{\mathcal{F}} \nabla \cdot (\phi \nabla \phi) d^3x. \end{aligned}$$

By Gauss' theorem this last expression can be written as an integral over the surface $\mathcal{S}$ of the body,

$$\begin{aligned} T_{\mathcal{F}} &= \rho_F \int_{\mathcal{F}} \nabla \cdot (\phi \nabla \phi) d^3x \\ &= -\rho_F \int_{\mathcal{S}} \phi \nabla \phi \cdot \mathbf{n} dS = \rho_F v_n \int_{\mathcal{S}} \phi dS. \end{aligned}$$

Using Kirchhoff's form for the potential it is clear that kinetic energy is quadratic in the body angular and translational velocity. Thus, the total kinetic energy can be written as,

$$T_{\text{total}} = \frac{1}{2} \begin{bmatrix} \boldsymbol{\Omega} & \mathbf{v} \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{S} \\ \mathbf{S}^T & \mathbf{M} \end{bmatrix} \begin{bmatrix} \boldsymbol{\Omega} \\ \mathbf{v} \end{bmatrix},$$

where $\mathbf{I}$ is the sum of the body inertia matrix and the *added inertia* due to the fluid, $\mathbf{S}$ accounts for coupling terms, and $\mathbf{M}$ is the sum of the body mass matrix and the *added mass* due to the fluid. For simple body shapes, these added effects of the fluid can be computed analytically; see, e.g., [18]. For example, if the body is ellipsoidal and the body-fixed frame coincides with the principal axes of the ellipsoid, $\mathbf{M}$ and $\mathbf{I}$ are diagonal and $\mathbf{S} = \mathbf{0}$. Expressions for the entries of the diagonal matrices $\mathbf{M}$ and $\mathbf{I}$ can be found in [18].

Using the kinematic relations $\hat{\boldsymbol{\Omega}} = B^{-1}\dot{B}$ and $\mathbf{v} = B^{-1}\dot{x}$, the Lagrangian $L : TSE(3) \to \mathbb{R}$ is given by

$$L(g, \dot{g}) = \frac{1}{2} \begin{bmatrix} B^{-1}\dot{B} & B^{-1}\dot{x} \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{S} \\ \mathbf{S}^T & \mathbf{M} \end{bmatrix} \begin{bmatrix} B^{-1}\dot{B} \\ B^{-1}\dot{x} \end{bmatrix}.$$

And the reduced Lagrangian $\ell : \mathfrak{se}(3) \to \mathbb{R}$ is simply its restriction to $\mathfrak{se}(3)$

$$\ell(\xi) = L(e, \xi) = \frac{1}{2} \begin{bmatrix} \boldsymbol{\Omega} & \mathbf{v} \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{S} \\ \mathbf{S}^T & \mathbf{M} \end{bmatrix} \begin{bmatrix} \boldsymbol{\Omega} \\ \mathbf{v} \end{bmatrix} = \frac{1}{2} \langle\langle \xi, \xi \rangle\rangle .$$

Adjoint action of SE(3) and $\mathfrak{se}$(3). The adjoint action of $SE(3)$ on $\mathfrak{se}(3)$ is given by,

$$\mathrm{Ad}_g \, \xi = \begin{bmatrix} B & \mathbf{x} \\ \mathbf{0} & 1 \end{bmatrix} \begin{bmatrix} \widehat{\boldsymbol{\Omega}} & \mathbf{v} \\ \mathbf{0} & 0 \end{bmatrix} \begin{bmatrix} B^T & -B^T\mathbf{x} \\ \mathbf{0} & 1 \end{bmatrix} = \begin{bmatrix} B\widehat{\boldsymbol{\Omega}}B^T & -B\widehat{\boldsymbol{\Omega}}B^T\mathbf{x} + B\mathbf{v} \\ \mathbf{0} & 0 \end{bmatrix}$$

which can be written as an action on $\mathbb{R}^3 \times \mathbb{R}^3$ as,

$$\mathrm{Ad}_{(B,\mathbf{x})}(\boldsymbol{\Omega}, \mathbf{v}) = (B\boldsymbol{\Omega}, B\mathbf{v} - \widehat{B\boldsymbol{\Omega}}\mathbf{x}).$$

Further by identifying $\mathfrak{se}(3)$ with $\mathbb{R}^3 \times \mathbb{R}^3$ and using the standard dot product pairing, the coadjoint action on $\mathfrak{se}(3)^*$ has the expression

$$\mathrm{Ad}^*_{(B,\mathbf{x})^{-1}}(\boldsymbol{\Omega}, \mathbf{v}) = (B\boldsymbol{\Omega} + \widehat{\mathbf{x}}B\mathbf{v}, B\mathbf{v}).$$

The corresponding Lie bracket of $\mathfrak{se}(3)$ is given by,

$$\mathrm{ad}_{\xi_1}\xi_2 = \xi_1\xi_2 - \xi_2\xi_1 = \begin{bmatrix} [\widehat{\boldsymbol{\Omega}}_1, \widehat{\boldsymbol{\Omega}}_2] & \widehat{\boldsymbol{\Omega}}_1\mathbf{v}_2 - \widehat{\boldsymbol{\Omega}}_2\mathbf{v}_1 \\ \mathbf{0} & 0 \end{bmatrix},$$

which is the usual commutator bracket. Using the identification to $\mathbb{R}^3 \times \mathbb{R}^3$ this adjoint action of $\sim(3)$ on itself has the expression,

$$\mathrm{ad}_{(\boldsymbol{\Omega}_1,\mathbf{v}_1)}(\boldsymbol{\Omega}_2, \mathbf{v}_2) = (\widehat{\boldsymbol{\Omega}_1}\boldsymbol{\Omega}_2, \widehat{\boldsymbol{\Omega}_1}\mathbf{v}_2 - \widehat{\boldsymbol{\Omega}_2}\mathbf{v}_1).$$

Likewise, the coadjoint action of $\mathfrak{se}(3)$ on its dual has the expression

$$\mathrm{ad}^*_{(\boldsymbol{\Omega}_1,\mathbf{v}_1)}(\boldsymbol{\Omega}_2, \mathbf{v}_2) = (\widehat{\boldsymbol{\Omega}_2}\boldsymbol{\Omega}_1 + \widehat{\mathbf{v}_2}\mathbf{v}_1, \widehat{\mathbf{v}_2}\boldsymbol{\Omega}_1).$$

For more details on the geometry of $SE(3)$ the reader is referred to [36, §14.7].

6.2 Kirchhoff Equations on $\mathfrak{se}(3)$

Suppose the solid is ellipsoidal so that $\mathbf{M}$ and $\mathbf{I}$ are diagonal and $\mathbf{S} = \mathbf{0}$. The dynamics of an ellipsoidal body in an ideal fluid is described by the Kirchhoff equations. These are just the reduced HP equations on $SE(3) \times \mathfrak{se}(3) \times \mathfrak{se}(3)^*$ for this Lagrangian system. These equations are written down explicitly here. Let $(\boldsymbol{\Pi}, \mathbf{p})$ denote the body angular velocity vector associated with $\mu \in \mathfrak{se}(3)^*$. Then the LP equations can be written as,

$$\frac{d}{dt}(\boldsymbol{\Pi}, \mathbf{p}) = \mathrm{ad}^*_{(\boldsymbol{\Omega},\mathbf{v})}(\boldsymbol{\Pi}, \mathbf{p}) = (\widehat{\boldsymbol{\Pi}}\boldsymbol{\Omega} + \widehat{\mathbf{p}}\mathbf{v}, \widehat{\mathbf{p}}\boldsymbol{\Omega}).$$

The reduced Legendre transform (3.6.2) implies that,

$$\ell'((\boldsymbol{\Omega}, \mathbf{v})) = (\boldsymbol{\Pi}, \mathbf{p}),$$

which can be written in matrix form as,

$$\begin{bmatrix} \boldsymbol{\Pi} \\ \mathbf{p} \end{bmatrix} = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{M} \end{bmatrix} \begin{bmatrix} \boldsymbol{\Omega} \\ \mathbf{v} \end{bmatrix}.$$

Collecting these results the reduced HP equations (3.6.1)-(3.6.3) for a ellipsoidal body in an ideal fluid follow,

$$\dot{\mathbf{x}} = B\mathbf{v}, \tag{6.2.1}$$

$$\dot{B} = B\widehat{\boldsymbol{\Omega}}, \tag{6.2.2}$$

$$\begin{bmatrix} \boldsymbol{\Pi} \\ \mathbf{p} \end{bmatrix} = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{M} \end{bmatrix} \begin{bmatrix} \boldsymbol{\Omega} \\ \mathbf{v} \end{bmatrix}, \tag{6.2.3}$$

$$\dot{\boldsymbol{\Pi}} + \widehat{\boldsymbol{\Omega}}\boldsymbol{\Pi} + \widehat{\mathbf{v}}\mathbf{p} = 0, \tag{6.2.4}$$

$$\dot{\mathbf{p}} + \widehat{\boldsymbol{\Omega}}\mathbf{p} = 0. \tag{6.2.5}$$

Similar to Euler's equations, the last three equations do not involve the Lie group variables B and $\mathbf{x}$. To reconstruct the solution on $SE(3)$ from the solution on $\mathfrak{se}(3)$, the following initial value problem,

$$\dot{\mathbf{x}} = B\mathbf{v}, \quad \dot{B} = B\widehat{\boldsymbol{\Omega}}$$

is solved for $B \in \mathrm{SO}(3)$ and $\mathbf{x} \in \mathbb{R}^3$.

Conservation of spatial angular momentum. From (3.7.3) the preserved momentum map is given by,

$$J(g, \xi, \mu) \cdot x = \left\langle \mathrm{Ad}^*_{g^{-1}} \mu, x \right\rangle = \mathrm{Trace}\left[\mu_s^T x\right],$$

where

$$\mu_s = \mathrm{Ad}^*_{g^{-1}}\,\mu = \begin{bmatrix} \widehat{B\mathbf{\Pi} + \hat{x}B\mathbf{p}} & B\mathbf{p} \\ \mathbf{0} & 0 \end{bmatrix},$$

and hence, $(B\mathbf{\Pi} + \hat{x}B\mathbf{p}, B\mathbf{p})$ is the conserved momentum map.

6.3 TLN and FLV for Kirchhoff Equations

With the above identification the TLN algorithm for rigid body in an ideal fluid will be derived in detail. Carrying this procedure out for MLN and FLV is very similar and therefore omitted.

TLN is derived from,

$$-\mu_{k+1} + \mu_k + \frac{h}{2}\left(\mathrm{ad}^*_{\xi_k}\,\mu_k + \mathrm{ad}^*_{\xi_{k+1}}\,\mu_{k+1}\right) = 0.$$

Using the identification of $se(3)$ to $\mathbb{R}^3 \times \mathbb{R}^3$ given earlier, this expression can be expanded to give,

$$(\mathbf{\Pi}_{k+1}, \mathbf{p}_{k+1}) = (\mathbf{\Pi}_k, \mathbf{p}_k) + \frac{h}{2}\left(\mathrm{ad}^*_{(\mathbf{\Omega}_k, \mathbf{v}_k)}(\mathbf{\Pi}_k, \mathbf{p}_k) + \mathrm{ad}^*_{(\mathbf{\Omega}_{k+1}, \mathbf{v}_{k+1})}(\mathbf{\Pi}_{k+1}, \mathbf{p}_{k+1})\right).$$

This expression can be rewritten as,

$$\mathbf{\Pi}_{k+1} = \mathbf{\Pi}_k - \frac{h}{2}\left(\widehat{\mathbf{\Omega}_k}\mathbf{\Pi}_k + \widehat{\mathbf{\Omega}_{k+1}}\mathbf{\Pi}_{k+1}\right) - \frac{h}{2}\left(\widehat{\mathbf{v}_k}\mathbf{p}_k + \widehat{\mathbf{v}_{k+1}}\mathbf{p}_{k+1}\right), \tag{6.3.1}$$

$$\mathbf{p}_{k+1} = \mathbf{p}_k - \frac{h}{2}\left(\widehat{\mathbf{\Omega}_k}\mathbf{p}_k + \widehat{\mathbf{\Omega}_{k+1}}\mathbf{p}_{k+1}\right). \tag{6.3.2}$$

This difference scheme together with the cayley reconstruction equation defines TLN on $SE(3)$. Table 6.1 lists the defining difference schemes on the Lie algebra for the LN and FLV methods tested.

Table 6.1: **LN and FLV for Kirchhoff Equations.**

Method	Defining Difference Equation
TLN	$\mathbf{\Pi}_{k+1} = \mathbf{\Pi}_k - \frac{h}{2}\left(\widehat{\mathbf{\Omega}_k}\mathbf{\Pi}_k + \widehat{\mathbf{\Omega}_{k+1}}\mathbf{\Pi}_{k+1}\right) - \frac{h}{2}\left(\widehat{\mathbf{v}_k}\mathbf{p}_k + \widehat{\mathbf{v}_{k+1}}\mathbf{p}_{k+1}\right)$ $\mathbf{p}_{k+1} = \mathbf{p}_k - \frac{h}{2}\left(\widehat{\mathbf{\Omega}_k}\mathbf{p}_k + \widehat{\mathbf{\Omega}_{k+1}}\mathbf{p}_{k+1}\right)$
MLN	$\mathbf{\Pi}_{k+1} = \mathbf{\Pi}_k - h\widehat{\mathbf{\Omega}_{k+1/2}}\mathbf{\Pi}_{k+1/2} - h\widehat{\mathbf{v}_{k+1/2}}\mathbf{p}_{k+1/2}$ $\mathbf{p}_{k+1} = \mathbf{p}_k - h\widehat{\mathbf{\Omega}_{k+1/2}}\mathbf{p}_{k+1/2}$
FLV	$\mathbf{\Pi}_{k+1} = \mathbf{\Pi}_{k-1} - h\widehat{\mathbf{\Omega}_k}\left(\mathbf{\Pi}_{k+1/2} + \mathbf{\Pi}_{k-1/2}\right) - h\widehat{\mathbf{v}_k}\left(\mathbf{p}_{k+1/2} + \mathbf{p}_{k-1/2}\right)$ $\mathbf{p}_{k+1} = \mathbf{p}_{k-1} - h\widehat{\mathbf{\Omega}_k}\left(\mathbf{p}_{k+1/2} + \mathbf{p}_{k-1/2}\right)$

6.4 CAY for Kirchhoff Equations

Using the identification of $\mathfrak{se}(3)$ to $\mathbb{R}^3 \times \mathbb{R}^3$ given by,

$$\xi = \begin{bmatrix} \widehat{\mathbf{\Omega}} & \mathbf{v} \\ \mathbf{0} & 0 \end{bmatrix} \in \mathfrak{se}(3); \quad \widehat{\mathbf{\Omega}} \in so(3); \quad \mathbf{v} \in \mathbb{R}^3$$

the CAY method will be specialized to $SE(3)$.

The Cayley transform on $\mathfrak{se}(3)$ does lie in $SE(3)$. In particular, for $\xi = (\mathbf{\Omega}, \mathbf{v}) \in \mathfrak{se}(3)$,

$$\operatorname{cay}(\xi) = \begin{bmatrix} \operatorname{cay}(\mathbf{\Omega}) & \left(e - \frac{1}{2}\widehat{\mathbf{\Omega}}\right)^{-1}\mathbf{v} \\ \mathbf{0} & 1 \end{bmatrix} \tag{6.4.1}$$

Thus, (4.6.6) takes the following form,

$$\begin{aligned} g_k^{-1} g_{k+1} &= \operatorname{cay}(h\xi_k) \\ &= \begin{bmatrix} \operatorname{cay}(h\mathbf{\Omega}_k) & h\left(e - \frac{h}{2}\widehat{\mathbf{\Omega}_k}\right)^{-1}\mathbf{v}_k \\ \mathbf{0} & 1 \end{bmatrix} \end{aligned}$$

Setting $g_k = (B_k, \mathbf{x}_k)$, this equation implies that

$$g_{k+1} = \begin{bmatrix} B_k \operatorname{cay}(h\mathbf{\Omega}_k) & hB_k \left(e - \frac{h}{2}\widehat{\mathbf{\Omega}_k}\right)^{-1} \mathbf{v}_k + \mathbf{x}_k \\ \mathbf{0} & 1 \end{bmatrix}.$$

The following identity will be useful in writing down (4.6.8) for $SE(3)$,

$$\begin{aligned} \langle \xi^* \mu \xi^*, \eta \rangle &= \operatorname{Trace}\left[\widehat{\mathbf{\Omega}}\widehat{\mathbf{\Pi}}\widehat{\mathbf{\Omega}}\delta\widehat{\mathbf{\Omega}} + \mathbf{v}\mathbf{p}^T\widehat{\mathbf{\Omega}}\delta\widehat{\mathbf{\Omega}}\right] \\ &= -(\mathbf{\Omega}^T\mathbf{\Pi})(\mathbf{\Omega}^T\delta\mathbf{\Omega}) - \mathbf{p}^T\widehat{\mathbf{\Omega}}\widehat{\mathbf{v}}\delta\mathbf{\Omega} \\ &= \delta\mathbf{\Omega}^T\left[-(\mathbf{\Omega}^T\mathbf{\Pi})\mathbf{\Omega} - \widehat{\mathbf{v}}\widehat{\mathbf{\Omega}}\mathbf{p}\right] \end{aligned}$$

Using the identity above, it is clear that CAY takes the following form for the Kirchoff equations,

$$B_{k+1} = B_k \operatorname{cay}(h\mathbf{\Omega}_k), \tag{6.4.2}$$

$$\mathbf{x}_{k+1} = hB_k\left(e - h/2\widehat{\mathbf{\Omega}_k}\right)^{-1}\mathbf{v}_k + \mathbf{x}_k, \tag{6.4.3}$$

$$\begin{bmatrix} \mathbf{\Pi}_k \\ \mathbf{p}_k \end{bmatrix} = \begin{bmatrix} \mathbf{I}\mathbf{\Omega}_k \\ \mathbf{M}\mathbf{v}_k \end{bmatrix}, \tag{6.4.4}$$

$$\begin{aligned} \mathbf{\Pi}_{k+1} = \mathbf{\Pi}_k &- \frac{h}{2}\left(\widehat{\mathbf{\Omega}_k}\mathbf{\Pi}_k + \widehat{\mathbf{\Omega}_{k+1}}\mathbf{\Pi}_{k+1}\right) - \frac{h}{2}\left(\widehat{\mathbf{v}_k}\mathbf{p}_k + \widehat{\mathbf{v}_{k+1}}\mathbf{p}_{k+1}\right) \\ &+ \frac{h^2}{4}\left((\mathbf{\Omega}_k^T\mathbf{\Pi}_k)\mathbf{\Omega}_k - (\mathbf{\Omega}_{k+1}^T\mathbf{\Pi}_{k+1})\mathbf{\Omega}_{k+1}\right) \\ &+ \frac{h^2}{4}\left(\widehat{\mathbf{v}_k}\widehat{\mathbf{\Omega}_k}\mathbf{p}_k - \widehat{\mathbf{v}_{k+1}}\widehat{\mathbf{\Omega}_{k+1}}\mathbf{p}_{k+1}\right), \end{aligned} \tag{6.4.5}$$

$$\mathbf{p}_{k+1} = \mathbf{p}_k - \frac{h}{2}\left(\widehat{\mathbf{\Omega}_k}\mathbf{p}_k + \widehat{\mathbf{\Omega}_{k+1}}\mathbf{p}_{k+1}\right). \tag{6.4.6}$$

6.5 Coadjoint & Energy-Preserving Methods for Kirchhoff Equations

In order to write down the explicit coadjoint preserving method for $SE(3)$ one needs the exponential map on $SE(3)$ which can be written in terms of the exponential map on SO(3) as follows. The exponential of $\xi = (\mathbf{\Omega}, \mathbf{v}) \in \mathfrak{se}(3)$ is given by

$$\exp(\xi) = \begin{bmatrix} \mathbf{g} & \mathrm{dexp}_{\mathbf{\Omega}}(\mathbf{v})) \\ \mathbf{0} & 1 \end{bmatrix},$$

which has the expression

$$\exp(\widehat{\mathbf{\Omega}}, \mathbf{v}) = (\exp(\mathbf{\Omega}), \mathrm{dexp}_{\mathbf{\Omega}}(\mathbf{v})),$$

where $\mathrm{dexp}_{\mathbf{\Omega}} : \mathfrak{so}(3) \to \mathfrak{so}(3)$ is the right trivialized tangent of exp on SO(3).

The SW method specialized to the underwater vehicle takes the following form,

$$g_{k+1} = g_k \exp(\mathbf{\Theta}_k, \mathbf{w}_k) = (\exp(\mathbf{\Theta}_k), \mathbf{x}_k), \tag{6.5.1}$$

$$\begin{bmatrix} \mathbf{\Pi}_k \\ \mathbf{p}_k \end{bmatrix} = \begin{bmatrix} \mathbf{I}\mathbf{\Omega}_k \\ \mathbf{M}\mathbf{v}_k \end{bmatrix}, \tag{6.5.2}$$

$$(\mathbf{\Pi}_{k+1}, \mathbf{p}_{k+1}) = (\exp(-\mathbf{\Theta}_k)(\mathbf{\Pi}_k - \widehat{\mathbf{x}_k}\mathbf{p}_k), \exp(-\mathbf{\Theta}_k)\mathbf{p}_k)\,. \tag{6.5.3}$$

By designing the update in terms of the coadjoint orbit, this map is spatial angular momentum-preserving for arbitrary $(\mathbf{\Theta}_k, \mathbf{w}_k) \in \mathbb{R}^3 \times \mathbb{R}^3$.

The explicit coadjoint preserving method defines $(\mathbf{\Theta}_k, \mathbf{w}_k)$ to ensure second-order accuracy:

$$\mathbf{\Theta}_k = h\mathbf{\Omega}_k + \frac{h^2}{2}\dot{\mathbf{\Omega}}_k,$$
$$\mathbf{w}_k = h\mathbf{v}_k + \frac{h^2}{2}\dot{\mathbf{v}}_k.$$

The coadjoint and energy preserving method picks $\mathbf{\Theta}_k$ to satisfy conservation of energy. Let $\mathcal{H}_0$ be the energy at $k = 0$. As before an intermediate variable $\widetilde{\mathbf{\Theta}}_k$

and scalar algebraic energy constraint are introduced,

$$\begin{aligned}
2\mathcal{H}(\mathbf{\Theta}_k, \mathbf{w}_k) =& (\mathbf{\Pi}_k - \widehat{\mathbf{w}_k}\mathbf{p}_k)^T \exp(\mathbf{\Theta}_k)\mathbf{I}^{-1}\exp(-\mathbf{\Theta}_k)(\mathbf{\Pi}_k - \widehat{\mathbf{w}_k}\mathbf{p}_k) \\
&+ \mathbf{p}_k^T \exp(\mathbf{\Theta}_k)\mathbf{M}^{-1}\exp(-\mathbf{\Theta}_k)\mathbf{p}_k, \\
\widetilde{\mathbf{\Theta}}_k =& h\mathbf{\Omega}_k + \frac{h^2}{2}\dot{\mathbf{\Omega}}_k, \\
\widetilde{\mathbf{w}}_k =& h\mathbf{v}_k + \frac{h^2}{2}\dot{\mathbf{v}}_k.
\end{aligned}$$

The coadjoint and energy preserving update generalized to the Kirchhoff equations is given by:

$$(\mathbf{\Theta}_k, \mathbf{w}_k) = (\widetilde{\mathbf{\Theta}}_k, \widetilde{\mathbf{w}}_k) + \lambda(\mathcal{H}_\Theta(\widetilde{\mathbf{\Theta}}_k, \widetilde{\mathbf{w}}_k), \mathcal{H}_w(\widetilde{\mathbf{\Theta}}_k, \widetilde{\mathbf{w}}_k)), \quad \mathcal{H}(\mathbf{\Theta}_k, \mathbf{w}_k) = \mathcal{H}_0.$$

KR generalized to the Kirchhoff equations:

$$(\mathbf{\Theta}_k, \mathbf{w}_k) = \lambda(\widetilde{\mathbf{\Theta}}_k, \widetilde{\mathbf{w}}_k), \quad \mathcal{H}(\mathbf{\Theta}_k, \mathbf{w}_k) = \mathcal{H}_0.$$

Notice that the KR scheme determines λ by enforcing energy conservation which is satisfied if λ is a root of $f : \mathbb{R} \to \mathbb{R}$ defined as,

$$\begin{aligned}
f(\lambda) = & (\mathbf{\Pi}_k - \lambda\widehat{\widetilde{\mathbf{w}}_k}\mathbf{p}_k)^T \exp(\lambda\widetilde{\mathbf{\Theta}}_k)\mathbf{I}^{-1}\exp(-\lambda\widetilde{\mathbf{\Theta}}_k)(\mathbf{\Pi}_k - \lambda\widehat{\widetilde{\mathbf{w}}_k}\mathbf{p}_k) \\
& \mathbf{p}_k^T \exp(\lambda\widetilde{\mathbf{\Theta}}_k)\mathbf{M}^{-1}\exp(-\lambda\widetilde{\mathbf{\Theta}}_k)\mathbf{p}_k - \mathbf{\Pi}_k^T\mathbb{I}^{-1}\mathbf{\Pi}_k - \mathbf{p}_k^T\mathbb{M}^{-1}\mathbf{p}_k.
\end{aligned}$$

However, the condition for the existence of a nontrivial solution to, $f(\lambda) = 0$, is not met as in the free rigid body since f is no longer a periodic function in λ. Thus, Krysl's method does not extend to $SE(3)$ or for that matter any group in which the condition of solvability for λ is no longer satisfied.

The algorithms are summarized in the following table.

Table 6.2: **Coadjoint and Energy Methods for Kirchhoff Equations**

Method	Definition of Relative Rotation Vector
SW	$(\boldsymbol{\Theta}_k, \mathbf{w}_k) = \Big(h\boldsymbol{\Omega}_k + h^2/2\dot{\boldsymbol{\Omega}}_k, \mathbf{v}_k + h/2(\dot{\mathbf{v}}_k + \widehat{\boldsymbol{\Omega}_k}\mathbf{v}_k)\Big)$
SW⊥	$(\boldsymbol{\Theta}_k, \mathbf{w}_k) = (\widetilde{\boldsymbol{\Theta}}_k, \widetilde{\mathbf{w}}_k) + \lambda(\mathcal{H}_\Theta(\widetilde{\boldsymbol{\Theta}}_k, \widetilde{\mathbf{w}}_k), \mathcal{H}_w(\widetilde{\boldsymbol{\Theta}}_k, \widetilde{\mathbf{w}}_k)), \mathcal{H}(\boldsymbol{\Theta}_k, \mathbf{w}_k) = \mathcal{H}_0$
KR	$(\boldsymbol{\Theta}_k, \mathbf{w}_k) = \lambda(\widetilde{\boldsymbol{\Theta}}_k, \widetilde{\mathbf{w}}_k), \quad \mathcal{H}(\boldsymbol{\Theta}_k, \mathbf{w}_k) = \mathcal{H}_0$

6.6 Simulation Results for Kirchhoff Equations

As pointed out by Aref and Jones, a Poincaré section can be computed to analyze the chaotic dynamics of an underwater vehicle [1]. In the computations that follow, we follow their approach to computing a transversal section in the reduced space of an underwater vehicle. However, the main goal is to test how well the integrators capture the statistical features of the flow rather than analyze the chaotic dynamics in detail. For details on this the reader is referred to their paper [1].

In Fig. 6.6.1, a Poincaré section is computed using CAY, TLN, FLV and a standard fourth order accurate Runge-Kutta method (RK4) for a long duration integration. From the figure it is clear that all methods qualitatively capture the right phase space structures except RK4. This evidence demonstrates that FLV, TLN, and MLN possess the same structure-preserving properties as the variational scheme CAY. Among these structure-preserving methods, Fig. 6.6.2 shows that FLV is the most efficient in capturing the qualitative structure of the Poincaré section.

Computations uing the coadjoint-preserving schemes SW and SW⊥ were not included in these figures because the methods perform poorly in this example as indicated in Fig. 6.6.3. In particular, the figure shows that the coadjoint-preserving methods fail to capture the right structure of the Poincaré section even though they preserve the coadjoint orbits and or energy, and the time span of integration is about 100 times shorter.

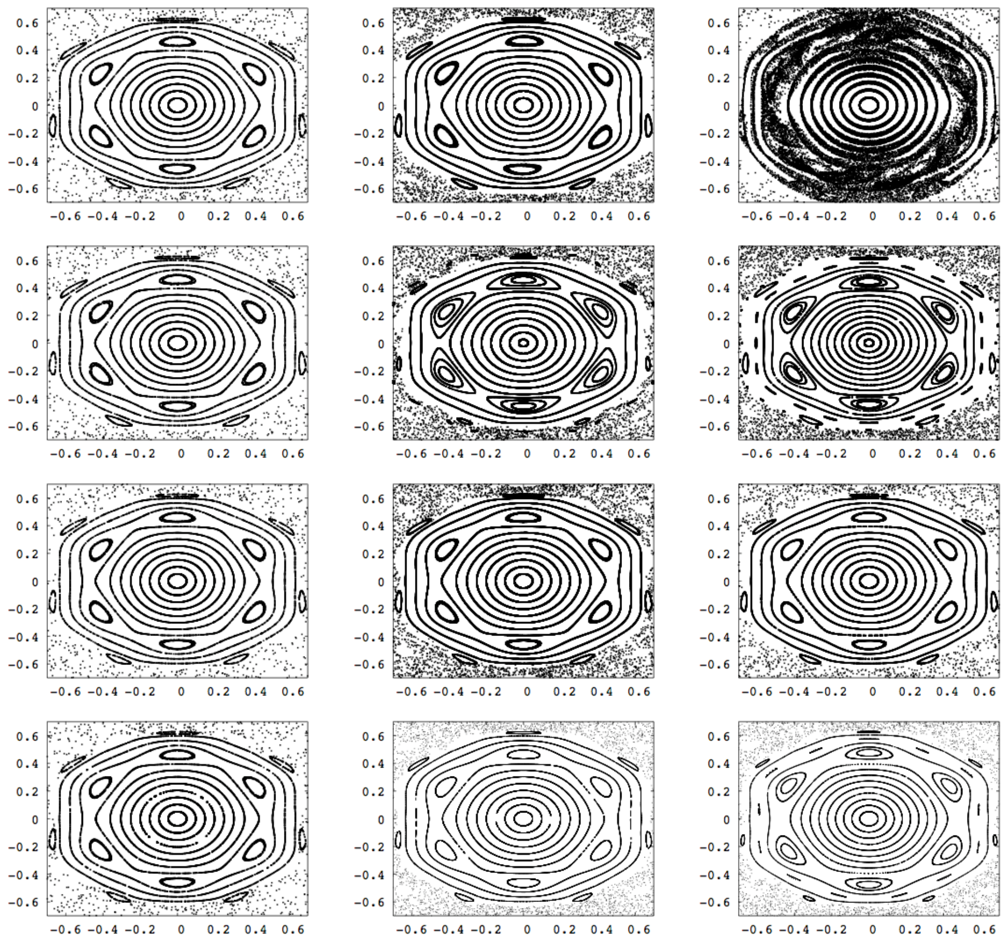


Figure 6.6.1: **Poincaré sections vs. Timestep.** From top Poincaré sections computed using RK4, CAY, TLN, and FLV. From left the timestep used is $h = 0.0125, 0.025, 0.05$ and the time-interval of integration is $[0, 10^6]$. These Poincaré sections are for a underwater vehicle with the following values of the integrals of motion $\mathbf{\Pi} \cdot \mathbf{p} = 0$, $\mathbf{p} \cdot \mathbf{p} = 5.2^2$ and $\mathcal{H} = 4.0$. The section is obtained by plotting points Π_x, Π_z for which $p_z = 0$. RK4 is the only method that does not perform well in this experiment.

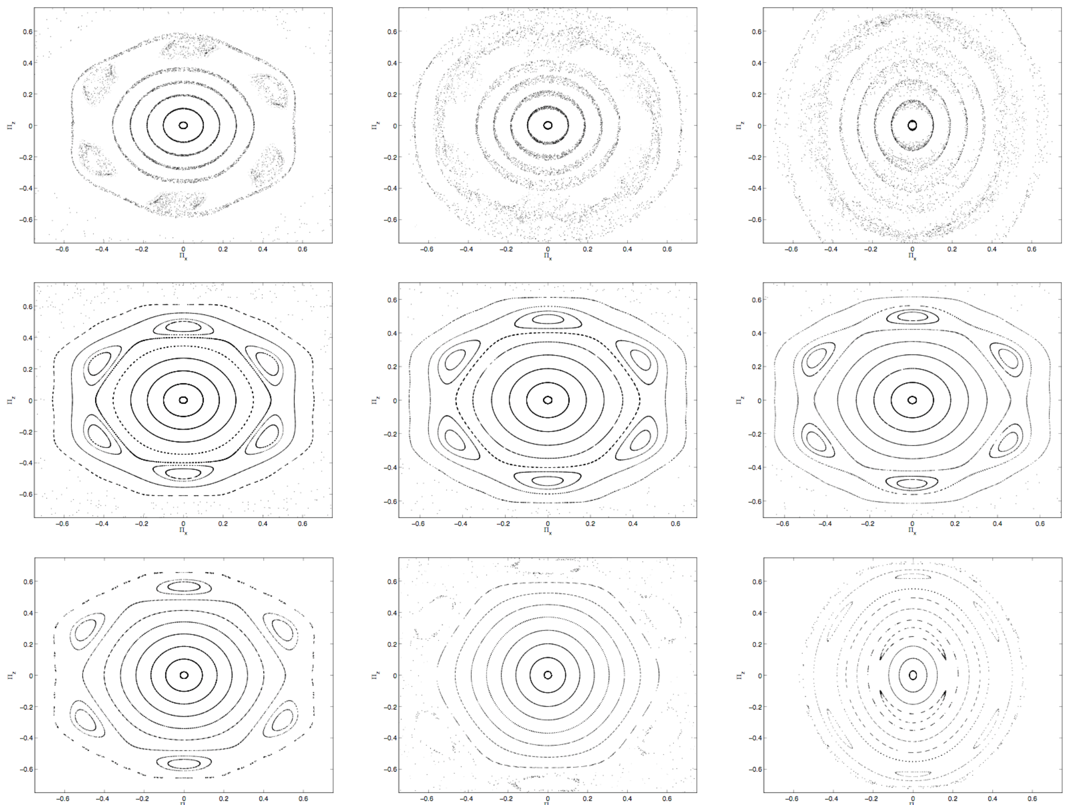


Figure 6.6.2: **Poincaré sections vs. CPU time.** From top Poincaré sections computed using RK4, FLV and MLN. From left the CPU-time used to produce the section is 20, 15, and 10 minutes and the time-interval of integration is $[0, 50000]$. These Poincaré sections are for a underwater vehicle with the following values of the integrals of motion $\mathbf{\Pi} \cdot \mathbf{p} = 0$, $\mathbf{p} \cdot \mathbf{p} = 5.2^2$ and $\mathcal{H} = 4.0$. The section is obtained by plotting points Π_x, Π_z for which $p_z = 0$. The top performer in capturing the qualitative dynamics of the flow in the time frame allotted is clearly FLV.

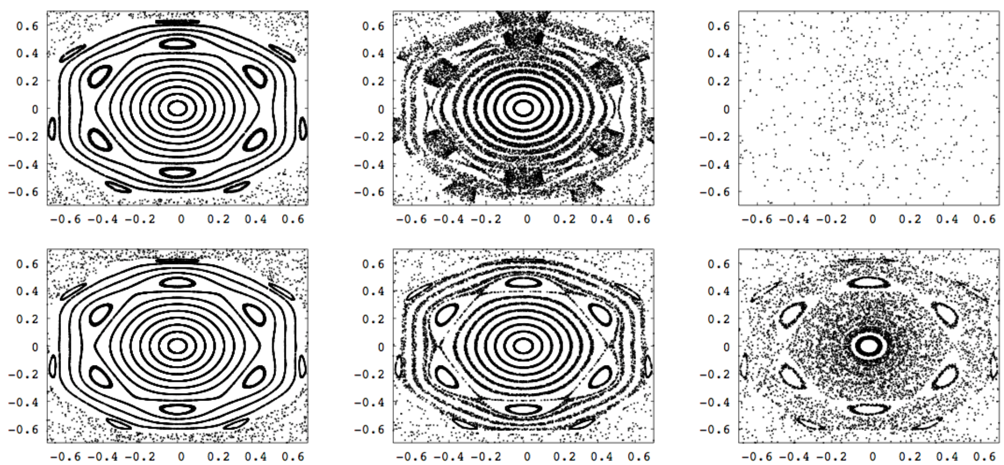


Figure 6.6.3: **Poincaré sections vs. Timestep.** From top Poincaré sections computed using SW and SW⊥. From left the timestep used is $h = 0.003125, 0.00625, 0.0125$ and the time-interval of integration is $[0, 50000]$. These Poincaré sections are for a underwater vehicle with the following values of the integrals of motion $\mathbf{\Pi} \cdot \mathbf{p} = 0$, $\mathbf{p} \cdot \mathbf{p} = 5.2^2$ and $\mathcal{H} = 4.0$. The section is obtained by plotting points Π_x, Π_z for which $p_z = 0$. At $h = 0.003125$ the methods capture the right dynamical behavior. However as h increases SW's performance drops even though it is preserving the coadjoint orbit. SW⊥ does marginally better since it also preserves energy.

Chapter 7

Applications, Future Directions/Vision

7.1 VPRK Integrators: The EP Case

The discrete HP principle states that the discrete path the discrete EP system takes is one that extremizes a reduced action sum that will be introduced shortly. To discretize the action integral, (4.2.5)-(4.2.6) are enforced as constraints by the introduction of internal and external stage Lagrange multipliers as shown in the definition below.

Definition 7.1.1. *Define the* ***discrete reduced VPRK path space****,*

$$\begin{aligned}\mathcal{C}_d(g_1, g_2) = \{(g, \mu, \{\Theta^i, \Xi^i, \Psi^i\}_{i=1}^s)_d : \{t_k\}_{k=0}^N \to (G \times \mathfrak{g}^*) \times (\mathfrak{g} \times \mathfrak{g} \times \mathfrak{g}^*)^s \mid \\ g(t_0) = g_1, \quad g(t_N) = g_2\}.\end{aligned}$$

and the ***reduced action sum*** $s_d : \mathcal{C}_d(g_1, g_2) \to \mathbb{R}$ *as*

$$\begin{aligned} s_d = \sum_{k=0}^{N-1} \sum_{i=1}^{s} h \Bigg[b_i \ell(\Xi_k^i) + \left\langle \Psi_k^i, \Theta_k^i/h - \sum_{j=1}^{s} a_{ij} d\tau^{-1}_{-\Theta_k^j} \Xi_k^j \right\rangle \\ + \left\langle \mu_{k+1}, \tau^{-1}(g_k^{-1} g_{k+1})/h - \sum_{j=1}^{s} b_j d\tau^{-1}_{-\Theta_k^j} \Xi_k^j \right\rangle \Bigg]. \end{aligned} \tag{7.1.1}$$

Observe that s_d is an approximation of the reduced HP action integral by numerical quadrature. The definition of τ as a map from $\mathfrak{g}$ to G ensures that the second pairing in the above sum is well defined. The discrete reduced HP principle states that,

$$\delta s_d = 0$$

for arbitrary and independent variations of the external stage vectors $(g_k, \mu_k) \in G \times \mathfrak{g}^*$ and the internal stage vectors $(\Theta_k^i, \Xi_k^i, \Psi_k^i) \in \mathfrak{g} \times \mathfrak{g} \times \mathfrak{g}^*$ for $i = 1, \cdots, s$ and $k = 0, \cdots, N$ subject to fixed endpoint conditions on $\{g_k\}_{k=0}^N$.

Theorem 7.1.2. *Let ℓ be a reduced Lagrangian on $\mathfrak{g}$ with continuous partial derivatives of second order with respect to its argument. A discrete curve $c_d \in \mathcal{C}_d(g_1, g_2)$ satisfies the following VPRK scheme:*

$$\begin{aligned}
\xi_{k+1} &= \textstyle\sum_{j=1}^s b_j d\tau^{-1}_{-\Theta_k^j} \Xi_k^j, \\
\Theta_k^i &= h \textstyle\sum_{j=1}^s a_{ij} d\tau^{-1}_{-\Theta_k^j} \Xi_k^j, \\
g_{k+1} &= g_k \tau(h\xi_{k+1}), \\
\Psi_k^i &= h(D(d\tau^{-1}_{-\Theta_k^i} \Xi_k^i))^* \left(\textstyle\sum_{j=1}^s a_{ji} \Psi_k^j + b_i \mu_{k+1} \right), \\
(d\tau^{-1}_{h\xi_{k+1}})^* \mu_{k+1} &= (d\tau^{-1}_{-h\xi_k})^* \mu_k, \\
b_i \ell'(\Xi_k^i) &= (d\tau^{-1}_{-\Theta_k^i})^* \left(\textstyle\sum_{j=1}^s a_{ji} \Psi_k^j + b_i \mu_{k+1} \right).
\end{aligned} \tag{7.1.2}$$

for $i = 1, \cdots, s$ and $k = 0, \cdots, N-1$, if it is a critical point of the function $s_d : \mathcal{C}_d(g_1, g_2) \to \mathbb{R}$, that is, $\mathbf{d}s_d(c_d) = 0$.

Proof. Let $\xi_{k+1} = \sum_{j=1}^s b_j d\tau^{-1}_{-\Theta_k^j} \Xi_k^j$. The variation of s_d with respect to the internal and external stage Lagrange multipliers imply the following difference equations are satisfied for $k = 0, \cdots, N-1$ and $i = 1, \cdots, s$,

$$\begin{aligned}
\delta\mu_{k+1} &\implies g_k^{-1} g_{k+1} = \tau(h\xi_{k+1}), \\
\delta\Psi_k^i &\implies \Theta_k^i = h \sum_{j=1}^s a_{ij} d\tau^{-1}_{-\Theta_k^j} \Xi_k^j.
\end{aligned}$$

These equations correspond to a s-stage RKMK discretization of the reconstruction equations.

For the variation with respect to Θ_k^i additional notation is introduced for the derivative of the right trivialized tangent of τ^{-1}, namely:

$$D(d\tau_\xi^{-1}\eta)\cdot\delta = \frac{\partial(d\tau_\xi^{-1}\eta)}{\partial\xi}\cdot\delta.$$

With this notation one can write

$$\delta\Theta_k^i \implies \Psi_k^i = h\sum_{j=1}^{s} a_{ji}(D(d\tau^{-1}_{-\Theta_k^i}\Xi_k^i))^*\Psi_k^j + b_i(D(d\tau^{-1}_{-\Theta_k^i}\Xi_k^i))^*\mu_{k+1}.$$

Factoring out $(D(d\tau^{-1}_{-\Theta_k^i}\Xi_k^i))^*$ gives,

$$\Psi_k^i = h(D(d\tau^{-1}_{-\Theta_k^i}\Xi_k^i))^*\left(\sum_{j=1}^{s} a_{ji}\Psi_k^j + hb_i\mu_{k+1}\right).$$

The variation with respect to Ξ_k^i yields,

$$\delta\Xi_k^i \implies b_i\ell'(\Xi_k^i) = \sum_{j=1}^{s} a_{ji}(d\tau^{-1}_{-\Theta_k^i})^*\Psi_k^j + b_i(d\tau^{-1}_{-\Theta_k^i})^*\mu_{k+1}$$

which can be rewritten to give the desired expression. Factoring out $(d\tau^{-1}_{-\Theta_k^i})^*$ gives,

$$b_i\ell'(\Xi_k^i) = (d\tau^{-1}_{-\Theta_k^i})^*\left(\sum_{j=1}^{s} a_{ji}\Psi_k^j + b_i\mu_{k+1}\right).$$

The variation of s_d with respect to g_k gives,

$$\delta g_k \implies \sum_{k=0}^{N-1}\left[\left\langle \mu_{k+1}, \delta\tau^{-1}(g_k^{-1}g_{k+1})\right\rangle\right] = 0.$$

Defining $\eta_k = g_k^{-1}\delta g_k$, and using the chain rule, one can write the above as

$$\sum_{k=0}^{N-1}\left[\left\langle \mu_{k+1}, \mathrm{D}\,\tau^{-1}(\tau(h\xi_{k+1}))\cdot(-TR_{\tau(h\xi_{k+1})}\eta_k + TL_{\tau(h\xi_{k+1})}\eta_{k+1})\right\rangle\right]h = 0.$$

In terms of the inverse right trivialized tangent, this can be written as

$$\sum_{k=0}^{N-1}\left[\left\langle \mu_{k+1}, d\tau^{-1}_{h\xi_{k+1}}(-\eta_k + \mathrm{Ad}_{\tau(h\xi_{k+1})}\,\eta_{k+1})\right\rangle\right] h = 0.$$

Summation by parts, the boundary conditions $\delta g_0 = \delta g_N = 0$, and lemma 4.1.6 imply that this can be rewritten as

$$\sum_{k=1}^{N-1}\left[\left\langle \mu_{k+1}, d\tau^{-1}_{h\xi_{k+1}}(-\eta_k)\right\rangle + \left\langle \mu_k, d\tau^{-1}_{-h\xi_k}(\eta_k)\right\rangle\right] h = 0.$$

Factoring out η_k gives

$$\sum_{k=1}^{N-1}\left[\left\langle -(d\tau^{-1}_{h\xi_{k+1}})^*\mu_{k+1} + (d\tau^{-1}_{-h\xi_k})^*\mu_k, \eta_k\right\rangle\right] h$$

which implies the following difference equation holds,

$$(d\tau^{-1}_{h\xi_{k+1}})^*\mu_{k+1} = (d\tau^{-1}_{-h\xi_k})^*\mu_k.$$

Keep in mind that $\xi_{k+1} = \sum_{j=1}^{s} b_j d\tau^{-1}_{-\Theta^j_k}\,\Xi^j_k$. These calculations complete the proof of the variational character of (7.1.2). ■

The external and internal stages of (7.1.2) define update schemes on $G \times \mathfrak{g}^*$ and $(\mathfrak{g} \times \mathfrak{g} \times \mathfrak{g}^*)^s$, respectively.

7.2 Order Conditions

In this section the global error of VPRK integrators will be examined. The section contains two theorems on the order of accuracy of VPRK integrators associated with a two- and three-stage Runge-Kutta approximation of the kinematic constraint. We arrive at order conditions by comparing the Taylor expansion of the exact solution to (3.6.1)-(3.6.3) and the numerical approximant generated by a VPRK integrator. Suppose that $g_k = g(t_k)$, $\xi_k = \xi(t_k)$, and $\mu_k = \mu(t_k)$ are exact.

Then the Taylor expansion of the exact solution about t_k for h small is given by:

$$\mu(t_k+h) = \mu_k + h\,\mathrm{ad}^*_{\xi_k}\mu_k + \frac{h^2}{2}\left(\mathrm{ad}^*_{\xi_k}\mathrm{ad}^*_{\xi_k}\mu_k + \mathrm{ad}_{\dot{\xi}_k}\mu_k\right) + \frac{h^3}{6}\left(2\,\mathrm{ad}^*_{\dot{\xi}_k}\mathrm{ad}^*_{\xi_k}\mu_k + \mathrm{ad}^*_{\xi_k}\mathrm{ad}^*_{\dot{\xi}_k}\mu_k + \mathrm{ad}^*_{\ddot{\xi}_k}\mu_k + \mathrm{ad}^*_{\xi_k}\mathrm{ad}^*_{\xi_k}\mathrm{ad}^*_{\xi_k}\mu_k\right) + \mathcal{O}(h^4),$$

and,

$$g(t_k+h) = g_k + hg_k\xi_k + \frac{h^2}{2}\left(g_k\xi_k^2 + g_k\dot{\xi}_k\right) + \frac{h^3}{6}\left(g_k\xi_k^3 + g_k\dot{\xi}_k\xi_k + 2g_k\xi_k\dot{\xi}_k + g_k\ddot{\xi}_k\right) + \mathcal{O}(h^4).$$

We now derive sufficient conditions for VPRK integrators to be second and third order accurate.

Conditions for order two. To design a method of second order, we pick the Euler-MK discretization of the reconstruction equation. In this case the VPRK simplifies to:

$$\begin{aligned} g_{k+1} &= g_k\tau(h\Xi_k) \\ (d\tau^{-1}_{h\Xi_k})^*\mu_{k+1} &= (d\tau^{-1}_{h\Xi_{k-1}})^*\mu_k \\ \ell'(\Xi_k) &= \mu_{k+1} \end{aligned} \tag{7.2.1}$$

which we refer to as the *variational Euler integrator*. The geometric properties of this scheme for various τ were analyzed in depth in Chapter 4.

7.3 Multiple Bodies with Orientation and Position-Dependent Potential

Continuous Description. Consider a mechanical system consisting of N rigid bodies interacting via a pairwise potential dependent on their positions and orientations. Let $(x_i(t), v_i(t), R_i(t), \omega_i(t)) \in TSE(3)$ denote the translational position, translational velocity, orientation, and spatial angular velocity of body i where i ranges from 1 to N. Let m_i and $\mathbb{I}_i$ denote the mass of body i and the diagonal inertia tensor of body i. The Lagrangian for the system is given by:

$$\ell(x_i, v_i, R_i, \omega_i) = \sum_{i=1}^{N} \frac{m_i}{2} v_i^{\mathrm{T}} v_i + \frac{1}{2} \omega_i^{\mathrm{T}} R_i \mathbb{I}_i R_i^{\mathrm{T}} \omega_i - U(x_i, R_i).$$

Note that $\ell(x_i, v_i, R_i, \omega_i)$ is shorthand notation for $\ell(x_1, v_1, R_1, \omega_1, \cdots, x_N, v_N, R_N, \omega_N)$. The path that the continuous system takes on the time-interval $[a, b]$ is one that extremizes the Hamilton-Pontryagin action:

$$s = \int_a^b \left[\ell(x_i, v_i, R_i, \omega_i) + \sum_{i=1}^{N} \langle p_i, \dot{x}_i - v_i \rangle + \left\langle \widehat{\pi}_i, \dot{R}_i R_i^{-1} - \widehat{\omega}_i \right\rangle \right] dt$$

for arbitrary variations with fixed endpoints: $(x_i(a), R_i(a))$ and $(x_i(b), R_i(b))$. The corresponding equations of motion are given by:

$$\begin{aligned}
\dot{x}_i &= v_i && \text{(reconstruction equation)}, \\
\dot{p}_i &= -U_{x_i} && \text{(Euler-Lagrange equations)}, \\
p_i &= m_i v_i && \text{(Legendre transform)}, \\
\dot{R}_i &= \widehat{\omega}_i R_i && \text{(reconstruction equation)}, \\
\dot{\pi}_i &= -U_{R_i} && \text{(Lie-Poisson equations)}, \\
\dot{\pi}_i &= R_i \mathbb{I}_i R_i^{\mathrm{T}} \omega_i && \text{(reduced Legendre transform)}.
\end{aligned}$$

The terms U_{x_i} and U_{R_i} are defined in terms of the inner product on $\mathbb{R}^3$ as,

$$\begin{aligned}
U_{x_i}^{\mathrm{T}} y &= \left\langle \frac{\partial U}{\partial x_i}, y \right\rangle = \partial_{x_i} U(x_i, R_i) \cdot y, \\
U_{R_i}^{\mathrm{T}} y &= \left\langle \frac{\partial U}{\partial R_i} R_i^{\mathrm{T}}, \widehat{y} \right\rangle = \partial_{R_i} U(x_i, R_i) \cdot \widehat{y} R_i,
\end{aligned}$$

where $\partial_{R_i} U : \mathrm{SO}(3) \to T_{R_i}^* \mathrm{SO}(3)$, and $\partial_{x_i} U : \mathbb{R}^3 \to T_{x_i}^* \mathbb{R}^3$ as defined below.

Variational integrator. For the discrete description, an extension of the variational Euler integrator provided in Chapter 4 is implemented. The action sum is given by

$$s_d = \sum_{k=0}^{N-1} h \left[\ell \left(x_i^{k+1}, v_i^{k+1}, R_i^{k+1}, \omega_i^{k+1} \right) + \left\langle p_i^{k+1}, (x_i^{k+1} - x_i^k)/h - v_i^{k+1} \right\rangle \right]$$
$$+ h \left[\left\langle \widehat{\pi_i^{k+1}}, \tau^{-1}(R_i^{k+1}(R_i^k)^{\mathrm{T}})/h - \widehat{\omega_i^{k+1}} \right\rangle \right].$$

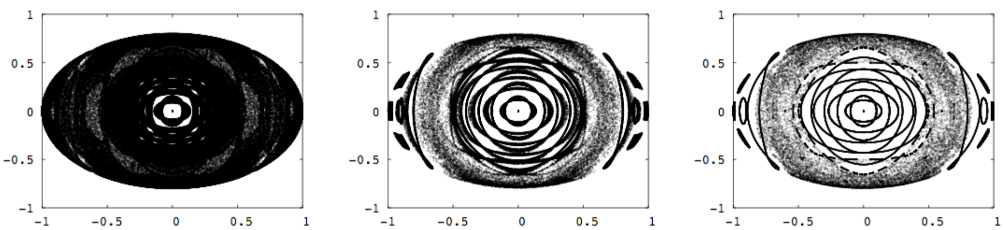
Let $d\tau^{-1}$ denote the right trivialized tangent of τ^{-1} as defined in Bou-Rabee & Marsden [2007]. Stationarity of this action sum implies the following discrete scheme:

$$\begin{aligned}
x_i^k &= x_i^{k-1} + h v_i^{k-1} && \text{(d. reconstruction equation)},\\
p_i^k &= p_i^{k-1} - h U_{x_i}(x_i^k, R_i^k) && \text{(d. Euler-Lagrange equations)},\\
p_i^k &= m v_i^k && \text{(d. Legendre transform)},\\
R_i^k &= \tau \left(\widehat{\omega_i^{k-1}} h \right) R_i^{k-1} && \text{(d. reconstruction equation)},\\
\left(d\tau^{-1}_{h\omega_i^k} \right)^* \pi_i^k &= \left(d\tau^{-1}_{h\omega_i^{k-1}} \right)^* \pi_i^{k-1} - h U_{R_i}(x_i^k, R_i^k) && \text{(d. Lie Poisson equation)},\\
\pi_i^k &= R_i^k \mathbb{I}_i (R_i^k)^{\mathrm{T}} \omega_i^k && \text{(d. reduced Legendre transform)}.
\end{aligned}$$

This integrator has the nice property that the translational and rotational configuration updates and the translational momentum update are explicit, i.e., one only has to perform an implicit solve for the discrete Lie-Poisson part. Even that computation is straightforward since the torque due to the potential is not a function of the angular velocity or momentum.

7.4 Mechanical Systems with Nontrivial Shape-Space Dynamics

A goal of future research is to generalize the HP integrators to Lagrange-Poincaré systems, i.e., Lagrangian systems whose configuration manifold is not necessarily a Lie group and whose Lagrangian is invariant with respect to the action of a Lie group. As explained below one can use a *connection*, a tool from geometric mechanics, to globally and intrinsically decompose the Euler-Lagrange equations on the tangent bundle into two reduced equations: Euler-Lagrange equations for the internal degrees of freedom and EP equations for the locked angular velocity with added effects to both equations due to the coupling between these spaces. Preliminary tests of the HP integrators to a Lagrange-Poincaré system with nontrivial internal shape space are encouraging: Fig. 7.4.1 displays the method's superior ability to compute a Poincaré section.



(a) SWb⊥, $h = 0.0625$ (b) RK4, $h = 0.25$ (c) HP Integrator, $h = 0.25$

Figure 7.4.1: **Rigid spacecraft with internal rotor and torsional spring.** From left: Poincaré sections computed using a coadjoint and energy-preserving method (SWb⊥), fourth order accurate Runge-Kutta (RK4) and FLV over the time-interval $[0, 10^6]$. The Poincaré section is a transversal plane in the vertical part of the reduced space of a rigid body with an internal rotor and torsional spring. FLV agrees with the benchmark and clearly preserves structure that RK4 and SWb⊥ do not.

Reduced Hamilton-Pontryagin (HP) principle. This principle as introduced in this thesis is useful in the design of reduced variational integrators because it does not involve restricted variations that usually appear in reduced variational principles [37; 9]. As a result the continuous principle becomes more transparent, and hence, one can see a wider range of discretizations such as a Cayley-based HP variational integrator derived and tested in the body. The vision here is to reduce the continuous HP principle in the Lagrange-Poincaré setting by extending Lagrangian reduction from Hamilton's principle as detailed in [9] to the HP principle. As explained below the mechanical connection plays an important role in this reduction process. This continuous theory will serve as a guide for the derivation of its discrete analog. With the discrete reduced HP principle, one could begin deriving and testing Lagrange-Poincaré integrators.

Mechanical connection. For a system of particles and rigid bodies, the mechanical connection enables one to split the tangent bundle (and variational principle) into a vertical and horizontal part [36]. Mechanically the vertical part represents the *locked angular velocity*, i.e., the angular velocity of the instantaneously equivalent rigid body obtained by locking the configuration of the system and the horizontal part represents the internal or shape space dynamics. From the split variational principle, two reduced equations arise: a vertical equation describing the evolution of the *locked angular velocity* and a horizontal equation describing the evolution on shape space, that are equivalent to the EP and Euler-Lagrange equations respectively with added effects due to the curvature of the connection. Using Routh rather than Lagrange-Poincaré reduction and the mechanical connection to derive reduced integrators, Jalnapurkar et al. showed that the connection is important in simulating systems with geometric phases because the reduced integrators avoid computing the complicated dynamics associated with the phases in the unreduced space [20]. By applying the Lagrange-Poincaré integrators to concrete examples, the precise role of the mechanical connection in the discrete theory and computation will be ascertained.

Examples. The discrete Lagrange-Poincaré theory can be numerically calibrated on the simple case of an Lagrange-Poincaré system with an abelian symmetry, e.g., a satellite rotating about an oblate Earth with an S^1 symmetry [20]. Once this trivial case has been vetted, one can test the Lagrange-Poincaré integrators on progressively more complicated Lagrange-Poincaré systems with non-abelian symmetry and ultimately to Argon 6 in a vacuum. Argon 6 is quite attractive to test on because it is known that the shape space geometry plays an important role in computing transition probabilities [50]. In fact, the reduction and efficient parametrization of shape space in terms of Jacobi vectors and the associated hyperspherical coordinates have already been worked out for this example. Thus, one can readily test the new Lagrange-Poincaré integrators on this system for relatively long time orbits that nonetheless play an important role in calculating these transition rates.

7.5 Stochastic Variational Integrators

Another goal of future research is to extend the methods from the thesis to the study of the nonequilibrium statistical properties of mechanical systems in isothermal environs. The strategy to do this is described in a very simple context, namely a sliding disk. This example is due to H. Owhadi, and will appear in a joint work [7].

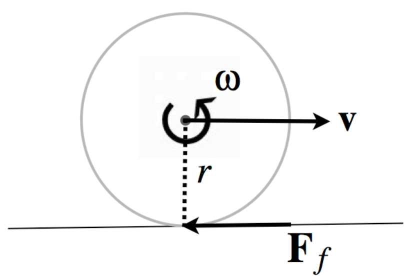


Figure 7.5.1: **Sliding disk.** Consider a sliding disk of radius r that is free to translate and rotate on a surface. We assume the disk is in sliding frictional contact with the surface.

Consider a disk on a surface as shown in Fig. 7.5.1. The disk is free to slide and rotate. Its Lagrangian is given by

$$L(x, v, \theta, \omega) = \frac{m}{2} v^2 + \frac{J}{2} \omega^2 - U(x)$$

where $U : \mathbb{R} \to \mathbb{R}$ is some potential which is assumed to be smooth. The contact with the surface is modelled using a sliding friction law. For this purpose we introduce a symmetric matrix $\mathbf{C}$ defined as,

$$\mathbf{C} = \begin{bmatrix} 1/m^2 & r/(mJ) \\ r/(mJ) & r^2/J^2 \end{bmatrix}.$$

Observe that $\mathbf{C}$ is degenerate since the frictional force is actually applied to only a single degree of freedom, and hence, one of its eigenvalues is zero. In addition to friction a noise parameter is introduced in the translational degree of freedom only. The dynamical equations for this mechanical system with noise and dissipation are

$$dx = vdt, \tag{7.5.1}$$

$$d\theta = \omega dt, \tag{7.5.2}$$

$$\begin{bmatrix} dv \\ d\omega \end{bmatrix} = \begin{bmatrix} -\partial_x U/m \\ 0 \end{bmatrix} dt - c\mathbf{C} \begin{bmatrix} mv \\ J\omega \end{bmatrix} dt + \alpha \begin{bmatrix} dB_v \\ 0 \end{bmatrix}. \tag{7.5.3}$$

Isothermal Sliding Disk The system (7.5.1)-(7.5.3) is put at constant temperature by modifying the noise term as described. Bou-Rabee & Owhadi prove that in a very precise sense the modified system is at a constant temperature given by $\beta = \alpha^2/2c$ [7]. This temperature is directly nonlinearly related to the amplitude α and inversely proportional to the friction factor c. The governing equations for the isothermal, sliding disk follow

$$dx = vdt, \tag{7.5.4}$$

$$d\theta = \omega dt, \tag{7.5.5}$$

$$\begin{bmatrix} dv \\ d\omega \end{bmatrix} = \begin{bmatrix} -\partial_x U/m \\ 0 \end{bmatrix} dt - c\mathbf{C} \begin{bmatrix} mv \\ J\omega \end{bmatrix} dt + \alpha\mathbf{C}^{1/2} \begin{bmatrix} dB_v \\ dB_\omega \end{bmatrix}, \tag{7.5.6}$$

where $\mathbf{C}^{1/2}$ is the matrix square root of $\mathbf{C}$. The matrix square root is easily computed by diagonalizing $\mathbf{C}$ and computing square roots of the diagonal entries (eigenvalues of $\mathbf{C}$) as shown:

$$\mathbf{C}^{1/2} = \begin{bmatrix} -\frac{mr}{J} & 1 \\ \frac{J}{mr} & 1 \end{bmatrix}^{-1} \begin{bmatrix} 0 & 0 \\ 0 & \sqrt{\frac{J^2+m^2r^2}{J^2m^2}} \end{bmatrix} \begin{bmatrix} -\frac{mr}{J} & 1 \\ \frac{J}{mr} & 1 \end{bmatrix} = \frac{1}{\sqrt{\frac{1}{m^2}+\frac{r^2}{J^2}}}\mathbf{C}.$$

The proof that this system is at constant temperature is based on finding the infinitesimal generator for (7.5.4)-(7.5.6) and showing that the Gibbs measure is invariant under the flow of this generator, and is the unique invariant measure of this system. It follows from this proof that the system is ergodic.

Stochastic HP integrator. To simulate the dynamics of the sliding disk at constant temperature, a stochastic variational Euler method is applied. In the limit as c and α tend to zero, the method limits to the usual variational Euler method which is the simplest symplectic partitioned Runge-Kutta method. In order to accelerate the computation, the nonconservative effects are lagged. To be specific, the discrete scheme for the isothermal case is given by:

$$x_{n+1} = x_n + hv_{n+1}, \tag{7.5.7}$$

$$\theta_{n+1} = \theta_n + h\omega_{n+1}, \tag{7.5.8}$$

$$\begin{bmatrix} v_{n+1} \\ \omega_{n+1} \end{bmatrix} = \begin{bmatrix} v_n \\ \omega_n \end{bmatrix} + h \begin{bmatrix} -\partial_x U(x_n)/m \\ 0 \end{bmatrix} - hc\mathbf{C} \begin{bmatrix} mv_n \\ J\omega_n \end{bmatrix} + \alpha \mathbf{C}^{1/2} \begin{bmatrix} dB_v \\ dB_\omega \end{bmatrix}. \tag{7.5.9}$$

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