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A Symplectic Integrator for Riemannian Manifolds

Ben Leimkuhler *
George W. Patrick **
[1] Department of Mathematics
University of Kansas
Lawrence, KS 660045
[2] Department of Mathematics and Statistics
University of Saskatchewan
Saskatoon, Saskatchewan, S7N 5E6
Canada

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Summary. The configuration spaces of mechanical systems usually support Riemannian metrics which have a explicitly solvable geodesic flows and parallel transport operators. While not of primary interest, such metrics can be used to generate integration algorithms by using the known parallel transport to evolve points in velocity phase space.

1. Introduction

There exist a number of mechanical systems having configuration and phase spaces that are differentiable manifolds which are not open subsets of Euclidean space. The spherical pendulum, which has configuration space the 2-sphere, and a single rigid body, with configuration space the Lie group $SO(3)$, are two common examples. Integration algorithms, on the other hand, are usually set in the Euclidean context. Use of a covering set of charts is straightforward in principle but can give unsatisfactory results in practice, since (i) it can increase the computational complexity of the algorithm, (ii) although a symplectic method can be used in each chart, between charts the discrete map changes, and this can lead to a systematic energy drift [6], and (iii) the numerical determination

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of when and how to switch charts can be complicated. If numerical computation must be done with tuples of floating point numbers, how can one proceed without charts?

This question has led to recent research on numerical methods that can be applied directly on various differential geometric objects. Such methods might be called *intrinsic*. Progress cannot be made strictly within the context of a manifold, symplectic or not: one requires the assistance of *some* global structure to construct *any* method. For example, McLachlan and Scovel [11] render configuration spaces as submanifolds of Euclidean space using global embeddings. From that point of view the mechanical system is a constrained system and the main issue is the finding of algorithms that map the constraint set to itself. One finds these ideas also in Barth and Leimkuhler [2] and Reich [14]. Crouch and Grossman [4] posit an independent spanning set of globally defined vector fields on phase space; the flows of these vector fields are used to move through phase space. Intrinsic Runge-Kutta methods, also using global vector fields, are investigated by Munthe-Kaas [12]. Lewis and Simo [7][8] have constructed conserving algorithms in the context of configuration spaces that are Lie groups, where a multitude of global objects are available.

Riemannian metrics are other global objects worthy of consideration when constructing intrinsic methods. Indeed, Riemannian geometry is a subject exactly invented to export common Euclidean notions to the global-manifold context. The main derived objects of a Riemannian metric are its geodesic flow and its parallel transport operators along geodesics. Riemannian geometry may be a promising base for numerical computation since many common diffeotypes of configuration spaces enjoy the presence of a Riemannian metric having explicitly known geodesic flow and parallel transport. Yet, no one seems to have used Riemannian geometry in the context of intrinsic integration algorithms.

In this article we show how such an ambient Riemannian metric can be used to frame the popular “leapfrog” method in the category of Riemannian manifolds, thus creating new intrinsic methods applicable to mechanical systems with configuration spaces as general as homogeneous spaces of semisimple Lie groups. This new method, shown in Figure (1), is implicit, second order, time-reversing, symplectic and respects those symmetries of the system which are also isometries of the ambient metric. For arbitrary potential energy, but where the kinetic energy metric of the mechanical system is proportional to the ambient metric, our method is *explicit*, and is equivalent to the splitting method corresponding to the splitting of the Hamiltonian into kinetic and potential energy.

2. Context and Notation

We will consider mechanical systems with configuration space Q, kinetic energy metric g, and potential V, so that the Lagrangian is

$$L(v_q) = \frac{1}{2}g(v_q, v_q) - V(q), \quad v_q \in T_qQ.$$

Given an initial state $tv_1 \in T_{q_1}Q$, find $w \in T_{q_1}Q$ by iterating

$$w = tv_1 - \frac{t^2}{2}\operatorname{grad}_g V(q_1) + \frac{1}{2}A(q_1, w),$$

where A is defined by

$$g^\flat(q_1)A(q_1,w) = \frac{1}{2}\tilde{\nabla} h(q_1)w^2 + h(q_1)\big(w, \tilde{\nabla}\Delta(q_2,q_1) + 2\mathrm{Id}\big) - h(q_2)\big(\mathbb{P}_{q_2}w, d\Delta(q_1,q_2)\big),$$

and $q_2 = \exp_{q_1} w$. The convergence of this step is faster for g nearer to $\tilde{g}$, and $A = 0$ for $g = \tilde{g}$, in which case this step is *explicit*. The new configuration is then

$$q_2 = \exp_{q_1} w.$$

The new state is $tv_2 \in T_{q_2}Q$, given by

$$tv_2 = \mathbb{P}_{q_2}w - \frac{t^2}{2}\operatorname{grad}_g V(q_2) + \frac{1}{2}A(q_2, -\mathbb{P}_{q_2}w).$$

If $(Q,\tilde{g})$ is a symmetric space, then

$$g^\flat(q_1)A(q_1,w) = \frac{1}{2}\tilde{\nabla} h(q_1)w^2 + h(q_1)\big(w, (2 - f_1/f_2)R_w\big) - h(q_2)\big(\mathbb{P}_{q_2}w, (1/f_2)R_w\big)$$

where R_w is the curvature operator of $\tilde{g}$, and f_1 and f_2 are the power series

$$f_1(z) = \cos\sqrt{z} = \sum_{k=0}^{\infty}\frac{(-1)^k}{(2k)!}z^k, \qquad f_2(z) = \frac{\sin\sqrt{z}}{\sqrt{z}} = \sum_{k=0}^{\infty}\frac{(-1)^k}{(2k+1)!}z^k.$$

Fig. 1. The algorithm.

Let a Lie group G act on Q by isometries with respect to g and suppose that V is G invariant. We will use the following standard notations [1]:

$$g^\flat : TQ \to T^\star Q \quad \langle g^\flat(v_q), w_q\rangle = g(q)(v_q, w_q),$$
$$g^\sharp : T^\star Q \to TQ \quad g^\sharp = (g^\flat)^{-1},$$
$$\operatorname{grad}_g V = g^\sharp \circ dV.$$

In other words, $g^\flat$ is the Legendre transformation, $g^\sharp$ is its inverse, and $-\operatorname{grad}_g V$ the force field divided by the "inertia".

Suppose that $f(q_1,q_2)$ is a differentiable function on $Q \times Q$. We use the notations $d_1 f$ and $d_2 f$ for the differential of f in its first and second argument, respectively. Thus, if $q_1(\epsilon)$ is a curve in Q, then

$$\left.\frac{d}{d\epsilon}\right|_{\epsilon=0} f\big(q_1(\epsilon)\big), q_2) = d_1 f\big(q_1(0), q_2\big)q_1'(0).$$

Suppose that $\tilde{g}$ is another metric on Q, and that the action of G on Q is isometric with respect to $\tilde{g}$. We think of the Riemannian geometry defined by $\tilde{g}$ as being known.

It may be helpful to keep in mind the following example: a particle of mass m moves on the ellipsoid

$$\frac{{y_1}^2}{{a_1}^2}+\frac{{y_2}^2}{{a_2}^2}+\frac{{y_3}^2}{{a_3}^2}=1$$

in the presence of some potential V, say $V=\mu y_3$, where μ is constant. The diffeotype of the ellipsoid is of course a 2-sphere, and transformation can be made to the 2-sphere by

$$x_1=\frac{y_1}{a_1},\quad x_2=\frac{y_2}{a_2},\quad x_3=\frac{y_3}{a_3}.$$

Through this transformation, the kinetic energy metric becomes

$$g=m{a_1}^2dx_1\otimes dx_1+m{a_2}^2dx_2\otimes dx_2+m{a_3}^2dx_3\otimes dx_3$$

(meaning the restriction of this to the unit 2-sphere) while the potential energy becomes $V=a_3\mu x_3$. If $a_1=a_2$ then the system admits the S^1 symmetry of rotations about the y_3 axis, and one can take the Lie group G to be S^1. The other metric $\tilde{g}$ is of course

$$\tilde{g}=dx_1\otimes dx_1+dx_2\otimes dx_2+dx_3\otimes dx_3.$$

The geometry generated by this metric (spherical geometry) is well known, and many elements of that geometry have well known closed formulas. Using the approach developed in this article, the geometry of $\tilde{g}$ can be used to navigate directly on the unit 2-sphere; preservation of constraint ${x_1}^2+{x_2}^2+{x_3}^2=1$ will not be an issue.

The exponential mapping of $\tilde{g}$ will be denoted exp, so that the geodesic starting at $q\in Q$ with velocity $v\in T_qQ$ is $\exp_q(tv)$. Parallel translation with respect to $\tilde{g}$ will be denoted by $\mathbb{P}$. Various forms will be used and the distinction will be clear from context. For example, if $q_1,q_2\in TQ$, $\mathbb{P}_{q_2,q_1}$ is the parallel translation operator along a previously defined curve joining q_1 to q_2, usually a geodesic. Sometimes q_1 is omitted. If $w\in TQ$, the notation $\mathbb{P}_w$ denotes the parallel translation operator along the geodesic curve $\exp(tw)$, $t\in[0,1]$. The covariant dervative of a vector field X on Q in the direction $v\in TQ$ is denoted by ∇_vX and satisfies (or is defined by, depending on how the theory is revealed)

$$\nabla_vX(q)=\left.\frac{d}{d\epsilon}\right|_{\epsilon=0}\mathbb{P}_qX(q+\epsilon v)$$

where $q+\epsilon v$ is any curve in ϵ with derivative v at $\epsilon=0$ and the parallel transport can be along the reverse of that curve. Covariant derivatives of other types of tensors satisfy (or are defined by) analogous formulas.

3. The Coordinate Version, Constant Metric

In this section we derive a special case of our algorithm, in order that it is introduced in a universally understood context. On the way, we show that, in this case, our algorithm reduces to the well known leapfrog algorithm. Specifically, we assume that $Q = \{q^i\}$ is an open subset of Euclidean space. The algorithm will be constructed on the assumption that g is constant. The metric $\tilde{g}$ does not make an appearance here; effectively it is the ordinary Euclidean metric.

3.1. The Generating Function

We aim for a second order time reversing algorithm, in part so that the Yoshida trick [15] can be applied. For a second order algorithm from a generating function of type 1, the appropriate generating function is [13]

$$\begin{aligned} S^1_t(q_1, q_2) \equiv \frac{1}{2t}&\left(g_{ij}(q_1)\Delta q^{ij} + \frac{1}{2} g_{ij;k}(q_1)\Delta q^{ijk}\right) \\ &- t\left(V(q_1) + \frac{1}{2}V_{;i}(q_1)\Delta q^i\right) \end{aligned} \quad (1)$$

where

$$\Delta q^{i_1\cdots i_n} = (q_2^{i_1} - q_1^{i_1})(q_2^{i_2} - q_1^{i_2})\cdots(q_2^{i_n} - q_1^{i_n}), \quad (2)$$

and $;i$ denotes differentiation by q^i. This generating function is defective since it is not symmetric in q_1 and q_2, and hence does not produce a time reversing algorithm. To remedy this, one can symmetrize:

$$\frac{1}{2}\big(S^1_t(q_1, q_2) + S^1_t(q_2, q_1)\big) = \frac{1}{4t}A_1 - \frac{t}{2}A_3,$$

where

$$A_1 \equiv \big(g_{ij}(q_1) + g_{ij}(q_2)\big)\Delta q^{ij} + \frac{1}{2}\big(g_{ij;k}(q_1) - g_{ij;k}(q_2)\big)\Delta q^{ijk}$$

and

$$A_3 \equiv \big(V(q_1) + V(q_2)\big) + \frac{1}{2}\big(V_{;i}(q_1) - V_{;i}(q_2)\big)\Delta q^i.$$

By [13], we may retain an order 2 algorithm by discarding terms in A_1 with up to third order derivatives in q_1 and q_2 zero at $q_1 = q_2$ and terms in A_3 with up to first order derivatives in q_1 and q_2 zero at $q_1 = q_2$. Thus, the second summands in both A_1 and A_3 may be discarded, and the generating function

$$S^2_t \equiv \frac{1}{4t}\big(g_{ij}(q_1) + g_{ij}(q_2)\big)\Delta q^{ij} - \frac{t}{2}\big(V(q_1) + V(q_2)\big) \quad (3)$$

defines an order 2 algorithm which is time reversible.

3.2. The Algorithm

The algorithm takes a point (q,p) in canonical phase space and advances by time t to obtain a point (q',p'). The point (q',p') is found by first solving the equation

$$p_k = -\frac{\partial S_t^2}{\partial q_1^k}(q,q') \tag{4}$$

for q' and then calculating

$$p'_k = \frac{\partial S_t^2}{\partial q_2^k}(q,q'). \tag{5}$$

Assuming constant g_{ij}, (4) takes the form

$$-p_k = -\frac{1}{t} g_{ik}\Delta q^i - \frac{t}{2} V_{;k}(q),$$

which has the solution

$$\Delta q^i = t g^{ik} p_k - \frac{t^2}{2} g^{ik} V_{;k}(q),$$

or by setting $v^i = g^{ik} p_k$,

$$q' = q + tv - \frac{t^2}{2} g^{-1}\nabla V(q), \tag{6}$$

where ∇ denotes the common gradient and g is the matrix with entries g_{ij}. Equation (5) becomes

$$\begin{aligned} p'_k &= \frac{1}{t} g_{ik}\Delta q^i - \frac{t}{2} V_{;k}(q') \\ &= p_k - \frac{t}{2}\big(V_{;k}(q) + V_{;k}(q')\big) \end{aligned}$$

or

$$p' = p - \frac{t}{2}\big(\nabla V(q) + \nabla V(q')\big). \tag{7}$$

The algorithm defined by (6) and (7) is the leapfrog algorithm as follows. Starting from the point $\big(q_0, p_{-\frac{1}{2}}\big)$, the leapfrog algorithm advances to the point $\big(q_1, p_{\frac{1}{2}}\big)$ by

$$p_{\frac{1}{2}} = p_{-\frac{1}{2}} - t\nabla V\big(q_0\big) \tag{8}$$

$$q_1 = q_0 + t g^{-1} p_{\frac{1}{2}}. \tag{9}$$

The next step advances $p_{\frac{1}{2}}$ to $p_{\frac{3}{2}}$ by

$$p_{\frac{3}{2}} = p_{\frac{1}{2}} - t\nabla V\big(q_1\big). \tag{10}$$

Set

$$p_0 = \frac{p_{-\frac{1}{2}} + p_{\frac{1}{2}}}{2}, \quad p_1 = \frac{p_{\frac{1}{2}} + p_{\frac{3}{2}}}{2}. \tag{11}$$

Using (11) to eliminate $p_{-\frac{1}{2}}$ from (8) gives

$$p_{\frac{1}{2}} = p_0 - \frac{t}{2}\nabla V(q_0), \tag{12}$$

and substitution of (12) into (9) gives

$$q_1 = q_0 + tg^{-1}p_0 - \frac{t^2}{2}g^{-1}\nabla V(q_0). \tag{13}$$

Taking the average of (8) and (10) yields

$$p_1 = p_0 - \frac{t}{2}\left(\nabla V(q_0) + \nabla V(q_1)\right). \tag{14}$$

Since (13) and (14) are equivalent to (6) and (7), the algorithm from the generating function (10) is equivalent, for constant g_{ij}, to the leapfrog algorithm.

4. On a Riemannian Manifold

In this section we leave coordinates on Q behind, using instead the Riemannian geometry of the metric $\tilde{g}$. This is accomplished first by replacing coordinate dependent portions of the generating function (3) by intrinsic (in the $\tilde{g}$ geometry) objects. The algorithm itself is obtained using only intrinsic operations, such as the covariant derivative. The result is an algorithm that advances on Q using parallel translation in the $\tilde{g}$ geometry.

4.1. The Generating Function

The exponential of the standard metric on $\mathbb{R}^n$ is exactly $\exp_q v = q + v$. Given $q_1 \in \mathbb{R}^n$ and $q_2 \in \mathbb{R}^n$, the quantity $\Delta q \equiv q_2 - q_1$ is the tangent vector at q_1 which tells how to get to q_2 using a geodesic. The idea is to replace Δq^i in (3) with $\Delta(q_2, q_1)$, which is defined by the equation

$$\exp_{q_1} \Delta(q_2, q_1) = q_2. \tag{15}$$

We have that $\Delta(q_2, q_1)$ is the same as $\Delta(q_1, q_2, 1)$ of [13], so that $\Delta(q_2, q_1)$ is defined and smooth for q_2 near to q_1. We guess that the function

$$\begin{aligned} S_t^3 \equiv \frac{1}{4t}\Big(&g(q_1)\big(\Delta(q_2, q_1), \Delta(q_2, q_1)\big) + g(q_2)\big(\Delta(q_2, q_1), \Delta(q_2, q_1)\big)\Big) \\ &- \frac{t}{2}\Big(V(q_1) + V(q_2)\Big) \end{aligned} \tag{16}$$

generates an order 2 algorithm.

And it does. To check this, take any chart on Q, again with coordinates q^i. Let the Christoffel symbols for the metric $\tilde{g}$ be $\tilde{\Gamma}^i_{jk}$. Then

$$\left[\exp_{q_1} v\right]^i = {q_1}^i + v^i - \frac{1}{2}\tilde{\Gamma}^i_{ab}(q_1)v^a v^b + \cdots = q_2^i$$

gives

$$\big[\Delta(q_2, q_1)\big]^i = \Delta q^i + \frac{1}{2}\tilde{\Gamma}^i_{ab}(q_1)\Delta q^a \Delta q^b + O\big((\Delta q)^3\big), \tag{17}$$

where $O\big((\Delta q)^3\big)$ denotes a function that has up to second order derivatives in q_1 and q_2 zero at $q_1 = q_2$. Now substituting (17) into the first part of (16) gives

$$\begin{aligned}
&g(q_1)\big(\Delta(q_2, q_1), \Delta(q_2, q_1)\big) + g(q_2)\big(\Delta(q_2, q_1), \Delta(q_2, q_1)\big)\\
&\quad = g_{ij}(q_1)\left(\Delta q^i + \frac{1}{2}\tilde{\Gamma}^i_{ab}(q_1)\Delta q^a \Delta q^b\right)\left(\Delta q^j + \frac{1}{2}\tilde{\Gamma}^i_{cd}(q_1)\Delta q^c \Delta q^d\right)\\
&\qquad + g_{ij}(q_2)\left(-\Delta q^i + \frac{1}{2}\tilde{\Gamma}^i_{ab}(q_2)\Delta q^a \Delta q^b\right)\left(-\Delta q^j + \frac{1}{2}\tilde{\Gamma}^i_{cd}(q_2)\Delta q^c \Delta q^d\right)\\
&\qquad\quad + O\big((\Delta q)^4\big)\\
&\quad = \big(g_{ij}(q_1) + g_{ij}(q_2)\big)\Delta q^{ij}\\
&\qquad + \big(g_{ij}(q_1)\tilde{\Gamma}^i_{ab}(q_1) - g_{ij}(q_2)\tilde{\Gamma}^i_{ab}(q_2)\big)\Delta q^{iab} + O\big((\Delta q)^4\big)\\
&\quad = \big(g_{ij}(q_1) + g_{ij}(q_2)\big)\Delta q^{ij} + O\big((\Delta q)^4\big),
\end{aligned}$$

as required. Showing that the second part of (16) has the required order of contact with the second part of (3) is even easier.

4.2. The Algorithm

We begin by setting $h = g - \tilde{g}$, so that $g = \tilde{g} + h$. Then [13] writing $\Delta(q_2, q_1)^2$ for a pair of $\Delta(q_2, q_1)$, the generating function

$$S^4_t(q_1, q_2) \equiv \frac{1}{2t}\tilde{g}(q_1)\Delta(q_2, q_1)^2 = \frac{d(q_1, q_2)^2}{2t} = \frac{1}{2t}\tilde{g}(q_2)\Delta(q_1, q_2)^2$$

generates the geodesic flow of $\tilde{g}$, where $d(q_1, q_2)$ is the Riemannian distance between q_1 and q_2. Thus, the generating function (16) can be written as follows:

$$\begin{aligned}
S^3_t(q_1, q_2) &= \frac{1}{4t}\big(g(q_1)\Delta(q_2, q_1)^2 + g(q_2)\Delta(q_1, q_2)^2\big) - \frac{t}{2}\big(V(q_1) + V(q_2)\big)\\
&= \frac{1}{2t}\tilde{g}(q_1)\Delta(q_2, q_1)^2 - \frac{t}{2}\big(V(q_1) + V(q_2)\big) && (18)\\
&\qquad + \frac{1}{4t}\big(h(q_1)\Delta(q_2, q_1)^2 + h(q_2)\Delta(q_1, q_2)^2\big). && (19)
\end{aligned}$$

The algorithm from this generating function takes $\alpha^1 \in T^*_{q_1}Q$ to $\alpha^2 \in T^*_{q_2}Q$, defined by first solving

$$-\alpha^1 = d_1 S^3_t(q_1, q_2) \tag{20}$$

for q_2 and then setting

$$\alpha^2 = d_2 S^3_t(q_1, q_2). \tag{21}$$

In this discussion, we will think of q_2 as $\exp_{q_1} w$, where $w \in T_{q_1}Q$. Since S_t^4 does generate the geodesic flow, we have the identities

$$\tilde{g}^\flat(q_1)w = -d_1\left(\frac{1}{2t}\tilde{g}(q_1)\Delta(q_2,q_1)^2\right), \tag{22}$$

$$\mathbb{P}_{q_2}\tilde{g}^\flat(q_1)w = d_2\left(\frac{1}{2t}\tilde{g}(q_1)\Delta(q_2,q_1)^2\right). \tag{23}$$

Using (22), the implicit part (20) of the algorithm becomes

$$\begin{aligned}
-\alpha^1 &= -\frac{1}{t}\tilde{g}^\flat(q_1)w - \frac{t}{2}dV(q_1) \\
&\qquad + d_1\left(\frac{1}{4t}h(q_1)\Delta(q_2,q_1)^2 + \frac{1}{4t}h(q_2)\Delta(q_1,q_2)^2\right) \\
&= -\frac{1}{t}\tilde{g}^\flat(q_1)w - \frac{t}{2}dV(q_1) + \frac{1}{4t}\tilde{\nabla}h(q_1)w^2 \\
&\qquad + \frac{1}{2t}h(q_1)\big(w, \tilde{\nabla}\Delta(q_2,q_1)\big) + \frac{1}{2t}h(q_2)\big(-\mathbb{P}_{q_2}w, d\Delta(q_1,q_2)\big),
\end{aligned} \tag{24}$$

where (24) contains various linear operators defined as follows: for $v \in T_{q_1}Q$,

$$\tilde{\nabla}h(q_1)w^2 \cdot v \equiv \tilde{\nabla}_v h(q_1)w^2, \tag{25}$$

$$\tilde{\nabla}\Delta(q_2,q_1)\cdot v \equiv \tilde{\nabla}_v\big(q_1 \mapsto \Delta(q_2,q_1)\big), \tag{26}$$

$$d\Delta(q_1,q_2)\cdot v \equiv \left.\frac{d}{d\epsilon}\right|_{\epsilon=0}\Delta(q_1+\epsilon v, q_2). \tag{27}$$

Here $q_1 + \epsilon v$ is any curve in ϵ having derivative v at $\epsilon = 0$. Equation (24) is calculated in a way that separates, as much as possible, the Riemannian geometry of $\tilde{g}$ from the system dependent quantity h.

We wish to write (24) as an iterative procedure for calculating w, and that would be possible simply by isolating the term $\tilde{g}^\flat(q_1)w$. However, the sum of the last two terms of (24) can be expected to fall only linearly with w, and so the iterative procedure would converge just in the case that h is small in comparison to g. This can be seen by considering the approximations

$$d\Delta(q_1,q_2)v \approx v, \qquad \tilde{\nabla}_v\Delta(q_2,q_1) \approx -v, \tag{28}$$

and then the sum of the last two terms of (24) looks like

$$-\frac{1}{t}h(q_1)(w,\cdot).$$

We want an iterative procedure that converges whenever w is small (i.e. whenever q_1 and q_2 are close). So we replace the $\tilde{g}$ in the first term of (24) with $g - h$ to obtain

$$\begin{aligned}
-\alpha^1 &= -\frac{1}{t}g^\flat(q_1)w + \frac{1}{t}h(q_1)^\flat w - \frac{t}{2}dV(q_1) + \frac{1}{4t}\tilde{\nabla}h(q_1)w^2 \\
&\qquad + \frac{1}{2t}h(q_1)\big(w, \tilde{\nabla}\Delta(q_2,q_1)\big) + \frac{1}{2t}h(q_2)\big(-\mathbb{P}_{q_2}w, d\Delta(q_1,q_2)\big).
\end{aligned} \tag{29}$$

If we define the quantity $A(q_1, w)$ by

$$
\begin{aligned}
g^\flat(q_1)A(q_1,w) = {} & \\
& \frac{1}{2}\nabla h(q_1) w^2 \\
& + h(q_1)\big(w, \nabla\Delta(q_2,q_1) + 2\mathrm{Id}\big) - h(q_2)\big(\mathbb{P}_{q_2} w, d\Delta(q_1,q_2)\big), \quad (30)
\end{aligned}
$$

then (29) becomes

$$
-\alpha^1 = -\frac{1}{t} g^\flat(q_1) w - \frac{t}{2} dV(q_1) + g^\flat(q_1)\frac{1}{2t} A(q_1,w), \tag{31}
$$

and here the approximations (28) suggest that A falls quadratically with w. Isolating w in (31) and making the replacement $\alpha^1 = g^\sharp(q_1)v_1$ yields

$$
w = tv_1 - \frac{t^2}{2}\operatorname{grad}_g V(q_1) + \frac{1}{2}A(q_1,w), \qquad q_2 = \exp_{q_1} w. \tag{32}
$$

For the explicit part of the algorithm that corresponds to (21), we find, using (23) and the fact that interchanging q_1 and q_2 means replacing w with $-\mathbb{P}_{q_2} w$, that

$$
\begin{aligned}
\alpha^2 &= \frac{1}{t} g^\flat(q_2)\mathbb{P}_{q_2} w - \frac{t}{2} dV(q_2) \\
&\qquad + d_2\left(\frac{1}{4t} h(q_1)\Delta(q_2,q_1)^2 + \frac{1}{4t} h(q_2)\Delta(q_1,q_2)^2\right) \\
&= \frac{1}{t} g^\flat(q_2)\mathbb{P}_{q_2} w - \frac{t}{2} dV(q_2) + \frac{1}{2}A(q_2, -\mathbb{P}_{q_2} w).
\end{aligned}
$$

Therefore,

$$
v_2 = \frac{1}{t}\mathbb{P}_{q_2} w - \frac{t}{2}\operatorname{grad}_g V(q_2) + \frac{1}{2t}A(q_2, -\mathbb{P}_{q_2} w). \tag{33}
$$

We note that the parallel translations that occur in (32) and (33) only translate w along the geodesic $\exp_{q_1}(tw)$, an operation which is identical with following the geodesic flow of $\tilde{g}$. Consequently, the full parallel translation operators are not required for the algorithm. Moreover, if g and $\tilde{g}$ are proportional, then $A = 0$, and the algorithm is exactly the iteration of $F_{t/2}G_t F_{t/2}$, where F is the flow of the Hamiltonian consisting just of of the potential energy and G is the flow of the Hamiltonian consisting just of the kinetic energy.

4.3. Calculations on a Symmetric Riemannian Manifold

As is apparent, it is not sufficient merely to know the exponential mapping of $\tilde{g}$. Indeed, by (26) and (27), derivatives of the map Δ are required, and Δ, being defined by (15), is in turn the inverse of exp. Thus at least one derivative of exp is required, and the task of calculating $\nabla\Delta$ and $d\Delta$ immediately attracts attention.

In this regard, it is useful to consider *Jacobi fields* and the class of *symmetric Riemannian manifolds*. Let us summarize the relevant facts, for which a general reference is [5]. Let M be a Riemannian manifold and $p \in M$.

1. The curvature operators $R_w : T_pM \to T_pM$, $w \in T_pM$ are defined by
$$R_w(v) = R(v,w)w, \tag{34}$$
where R is the Riemann curvature tensor.
2. A Jacobi field over a geodesic $c(t)$ is a vector field $Y(t)$ over $c(t)$ satisfying
$$\frac{\nabla^2 Y}{dt^2} + R_{\dot{c}(t)}Y(t) = 0.$$
In appropriate coordinates, this is a non-autonomous second order linear ordinary differential equation, and so there is a unique Jacobi field $Y(t)$ for specified $Y(0)$ and $\nabla Y/dt(0)$.
3. Let $p + \epsilon a$ be any curve at p with derivative $a \in T_pM$ and let $b \in T_pM$. From page 113 of [5][3], the vector field
$$Y(t) = \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \exp_{p+\epsilon a}(\mathbb{P}_{p+\epsilon a} wt)$$
is the Jacobi field over $\exp_p(wt)$ such that
$$Y(0) = a, \qquad \frac{\nabla Y}{dt}(0) = 0,$$
and the vector field
$$Y(t) = \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \exp_p\big((w+\epsilon b)t\big)$$
is the Jacobi field over $\exp_p(wt)$ such that
$$Y(0) = 0, \qquad \frac{\nabla Y}{dt}(0) = b.$$
4. By definition, M is a symmetric space if it is connected and if for all $p \in M$ there is an isometry σ_p such that $\sigma_p(p) = p$ and $T_p\sigma_p = -\mathrm{Id}$.
5. Suppose M is a symmetric space, $v, w \in T_pM$. Then
$$\mathbb{P}_{vt} R_w = R_{\mathbb{P}_{vt} w} \mathbb{P}_{vt},$$
that is R is parallel, and
$$\mathbb{P}_v = T_p\big(\sigma_{\exp_p(v/2)} \circ \sigma_p\big). \tag{35}$$

[3] In [5] on page 113 the equation for A(t), which is the relevant one for what we require, is in error: A_0 and A_1 must be interchanged.

6. Suppose M is a symmetric space, and define the power series

$$f_1(z) = \cos\sqrt{z} = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k)!} z^k, \qquad f_2(z) = \frac{\sin\sqrt{z}}{\sqrt{z}} = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)!} z^k.$$

For $a, b \in T_p M$, the Jacobi field $Y(t)$ over $\exp_p(wt)$ such that

$$Y(0) = a, \qquad \frac{\nabla Y}{dt}(0) = b,$$

is

$$Y(t) = \mathbb{P}_{wt}\left(f_1(t^2 R_w)a + f_2(t^2 R_w)b\right).$$

We now calculate $d\Delta$. Let $q_1, q_2 \in Q$, $w = \Delta(q_2, q_1)$ and $\tilde{w} = \mathbb{P}_{q_2} w = -\Delta(q_1, q_2)$. Differentiating the defining equation of Δ, namely

$$\exp_{q_1} \Delta(q_2 + \epsilon v, q_1) = q_2 + \epsilon v, \qquad v \in T_{q_2} Q,$$

we obtain,

$$v = \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \exp_{q_1} \Delta(q_2 + \epsilon v, q_1) = \mathbb{P}_{q_2} f_2(R_w) d\Delta(q_2, q_1) v,$$

so that

$$d\Delta(q_2, q_1) v = \left(f_2(R_w)\right)^{-1} \mathbb{P}_{q_1} v = (1/f_2)(R_w) \mathbb{P}_{q_1} v. \tag{36}$$

Also, for $v \in T_{q_1} Q$,

$$\begin{aligned} d\Delta(q_1, q_2) v &= (1/f_2)(R_{-\tilde{w}}) \mathbb{P}_{q_2} v \\ &= \mathbb{P}_{q_2} \mathbb{P}_{q_1} (1/f_2)(R_{\tilde{w}}) \mathbb{P}_{q_2} v \\ &= \mathbb{P}_{q_2} (1/f_2)(R_w) v. \end{aligned} \tag{37}$$

The calculation of $\nabla\Delta$ is similar, starting with the equation

$$\exp_{q_1 + \epsilon v} \Delta(q_2, q_1 + \epsilon v) = q_2, \qquad v \in T_{q_1} Q,$$

and differentiating, we have

$$\begin{aligned} 0 &= \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \exp_{q_1+\epsilon v} \Delta(q_2, q_1 + \epsilon v) \\ &= \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \exp_{q_1+\epsilon v} \left(\mathbb{P}_{q_1+\epsilon v} \mathbb{P}_{q_1} \Delta(q_2, q_1 + \epsilon v)\right) \\ &= \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \exp_{q_1+\epsilon v} \left(\mathbb{P}_{q_1+\epsilon v} \mathbb{P}_{q_1} \Delta(q_2, q_1)\right) + \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \exp_{q_1} \left(\mathbb{P}_{q_1} \Delta(q_2, q_1 + \epsilon v)\right) \\ &= \mathbb{P}_{q_2}\left(f_1(R_w) v + f_2(R_w) \nabla_v \Delta(q_2, q_1)\right). \end{aligned}$$

Consequently,

$$\nabla_v \Delta(q_2, q_1) = -(f_1/f_2)(R_w) v \tag{38}$$

and for $v \in T_{q_2}Q$,

$$\nabla_v \Delta(q_1, q_2) = -\mathbb{P}_{q_2}(f_1/f_2)(R_w)\mathbb{P}_{q_1} v. \tag{39}$$

Note that since $f_1(z) = 1 + O(z)$ and $f_2(z) = 1 + O(z)$, the approximations (28) are confirmed by (37) and (38). Moreover, since R_w contains w twice, R_w falls quadratically with w. Thus, if the power series for $\nabla\Delta$ and $d\Delta$ are substituted into (30), then the terms that depend on R_w fall cubically with w, suggesting that R_w may not require recalculation on every iteration of (32).

5. Special Cases

5.1. On a 2-Sphere

Throughout this section, we will take

$$Q = \{q \in \mathbb{R}^3 \mid q \cdot q = a^2\}, \qquad \tilde{g}\big((q, v_1), (q, v_2)\big) = \mu^2 v_1 \cdot v_2,$$

where $a > 0$ and $\mu > 0$. We will use the standard identification of $\mathbb{R}^3$ and $so(3)$ by $v \in \mathbb{R}^3 \mapsto v^\wedge \in so(3)$ where

$$v^\wedge = \begin{bmatrix} 0 & -v^3 & v^2 \\ v^3 & 0 & -v^1 \\ -v^2 & v^1 & 0 \end{bmatrix}.$$

Note that $v^\wedge w = v \times w$. We will write the $SO(3)$-exponential mapping of $v \in so(3)$ as $\exp v^\wedge$.

The geodesic through $q \in Q$ in the direction of $v \in T_qQ$ is the great circle along v, so that

$$\exp_q v = \exp\left(\frac{1}{a^2}(q \times v)^\wedge\right) q. \tag{40}$$

By (35) or otherwise,

$$\mathbb{P}_v w = \exp\left(\frac{1}{a^2}(q \times v)^\wedge\right) w. \tag{41}$$

For $\nabla\Delta$ and $d\Delta$, we must calculate $(1/f_2)(R_w)$ and $(f_1/f_2)(R_w)$. From page 101 of [5],

$$R_w v = \frac{1}{a^2}\big(|w|^2 v - (v \cdot w)w\big), \tag{42}$$

and so

$$\begin{aligned} R_w^2 v &= \frac{1}{a^2} R_w \left(|w|^2 v - (v \cdot w)w\right) \\ &= \frac{1}{a^4}\Big(|w|^2\big(|w|^2 v - (v \cdot w)w\big) - \big(\big(|w|^2 v - (v \cdot w)w\big) \cdot w\big) w\Big) \\ &= \frac{|w|^2}{a^4}\big(|w|^2 v - (v \cdot w)w\big) \\ &= \frac{|w|^2}{a^2} R_w v. \end{aligned} \tag{43}$$

Now let $f(z)$ be a generic power series in z:

$$f(z) = \sum_{k=0} c_k z^k.$$

Using (43),

$$\begin{aligned} f(R_w) &= c_0 \mathrm{Id} + c_1 R_w + c_2 R_w^2 + c_3 R_w^3 \cdots \\ &= c_0 \mathrm{Id} + c_1 R_w + c_2 \frac{|w|^2}{a^2} R_w + c_3 \frac{|w|^4}{a^4} R_w + \cdots \\ &= f(0)\mathrm{Id} + \left(f\left(\frac{|w|^2}{a^2}\right) - f(0)\right) \frac{a^2}{|w|^2} R_w . \end{aligned}$$

Applying this to $(1/f_2)(z) = \sqrt{z}/\sin\sqrt{z}$ and to $(f_1/f_2)(z) = \sqrt{z}\cos\sqrt{z}/\sin\sqrt{z}$ yields

$$(1/f_2)(R_w) = \mathrm{Id} + g_1\left(\frac{|w|}{a}\right) R_w, \qquad (f_1/f_2)(R_w) = \mathrm{Id} + g_2\left(\frac{|w|}{a}\right) R_w,$$

where

$$g_1(z) = \frac{1}{z^2}\left(\frac{z}{\sin z} - 1\right), \qquad g_2(z) = \frac{1}{z^2}\left(\frac{z\cos z}{\sin z} - 1\right).$$

Care is required to avoid error in the numerical evaluation of these quantities, since $|w|$ is near zero. Recasting them as

$$g_1(z) = \left(\frac{z}{\sin z}\right)\left(\frac{z - \sin z}{z^3}\right)$$

and

$$\begin{aligned} g_2(z) &= \frac{1}{z^2 \sin z}(z\cos z - \sin z) \\ &= \frac{1}{z^2 \sin z}(z\cos z - z) + \frac{1}{z^2 \sin z}(z - \sin z) \\ &= \frac{1}{z\sin z}\frac{\cos^2 z - 1}{\cos z + 1} + g_1(z) \\ &= g_1(z) - \frac{\sin z}{z}\frac{1}{1+\cos z}, \end{aligned}$$

one sees that it is enough to be able to calculate

$$\frac{\sin z}{z} \quad \text{and} \quad \frac{\sin z - z}{z^3}$$

for small z.

For the calculation of $\nabla h(q)w^2$, we assume that all of g, $\tilde{g}$ and h are the restrictions of tensors (denoted by the same name) on an open subset of $\mathbb{R}^3$ containing Q. Then

$$\begin{aligned}\nabla_v h(w,w) &= \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} h(q+\epsilon v)\big(\mathbb{P}_{\epsilon v} w, \mathbb{P}_{\epsilon v} w\big) \\ &= \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} h(q+\epsilon v)\big(w,w\big) + \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} h(q)\big(\mathbb{P}_{\epsilon v} w, \mathbb{P}_{\epsilon v} w\big) \\ &= d\big(h(q)(w,w)\big)v + 2h\big(\Gamma(q,v)w, w\big)\end{aligned}$$

where $\Gamma(q,v)$ is

$$\begin{aligned}\Gamma(q,v) &= \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \exp\left(\frac{\epsilon}{a^2}(q\times v)^\wedge\right) w \\ &= \frac{1}{a^2}(q\times v)\times w \\ &= -\frac{1}{a^2}(w\cdot v)q.\end{aligned}$$

Thus,

$$\nabla h(q)w^2 = d\big(h(q)(w,w)\big) - \frac{1}{a^2}h(w, qw^T).$$

Finally, in the calculation of $\mathrm{grad}_g V$ and A, the map $g^\sharp$ is required. So suppose α is a covector in $\mathbb{R}^3$ (i.e. a row vector) representing a covector in Q by $v \mapsto \alpha v$ where $v \in T_qQ \Leftrightarrow v\cdot q = 0$. The vector $z = g^\sharp(\alpha)$ is characterized by $z\cdot q = 0$ and $g(q)(z,v) = \alpha v$ for all $v \cdot q = 0$. Let G be the matrix of the extension of g at q. Then we seek z such that

$$z^T G v = \alpha v, \quad z\cdot q = 0.$$

Trying $z^T G = \alpha + \gamma q^T$ for some $\gamma \in \mathbb{R}$ satisfies the first equation. Postmultiplication by G^{-1}, transposing, premultiplying by q^T, and using $z\cdot q = 0$ gives

$$\gamma = -\frac{\alpha G^{-1} q}{q^T G^{-1} q}.$$

Thus,

$$g^\sharp(\alpha) = \alpha - \frac{\alpha G^{-1} q}{q^T G^{-1} q} q.$$

5.2. On a Lie Group or Homogeneous Space

We begin with the specific case where Q is a Lie group upon which $\tilde{g}$ is an bi-invariant metric. Let the Lie algebra of Q be $\mathfrak{q}$. Denote the Lie group exponential mapping of Q by exp; it can be distinguished from the exponential mapping of the bi-invariant metric by context. Identify TQ with $Q\times\mathfrak{q}$ using left translations, so that

$$(q,\tilde{w}) \in Q\times\mathfrak{q} \equiv w = \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} q\exp(\tilde{w}\epsilon) = TL_q\tilde{w},$$

where L is the left multiplication mapping. Then we have the following, from Section (1.7) of [5] or Sections (7.8) and (8.3) of [3].

1. The exponential mapping of the bi-invariant metric is $\exp_q v = q \exp \tilde{v}$.
2. The mappings $\sigma_q x = qx^{-1}q$, $q \in Q$ are isometries making Q into a symmetric space.
3. Parallel translation along the geodesic $\exp_q(wt)$ is the derivative of the map

$$\begin{aligned} x \mapsto\ & \sigma_{\exp_q(w\epsilon/2)}\sigma_q x \\ &= \sigma_{q\exp(\tilde{w}\epsilon/2)} q x^{-1} q \\ &= q\exp(\tilde{w}\epsilon/2)q^{-1}xq^{-1}q\exp(\tilde{w}\epsilon/2) \\ &= q\exp(\tilde{w}\epsilon/2)q^{-1}x\exp(\tilde{w}\epsilon/2), \end{aligned}$$

   so that, remembering that the result is to be left translated to the identity, parallel translation becomes

$$\begin{aligned} \mathbb{P}_{tw} v &= TL_{(q\exp(\tilde{w}t))^{-1}} \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} q\exp(\tilde{w}t/2)q^{-1}\big(q\exp(\tilde{v}\epsilon)\big)\exp(\tilde{w}t/2) \\ &= \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \exp(-\tilde{w}t/2)\exp(\tilde{v}\epsilon)\exp(\tilde{w}t/2) \\ &= \mathrm{Ad}_{\exp(-\tilde{w}t/2)}\,\tilde{v}. \end{aligned}$$

   In particular, $\mathbb{P}_{tw} w = w$, so the parallel translations occuring in the algorithm do not change their arguments.
4. The curvature operator is given by $R_w = -\frac{1}{4}\,\mathrm{ad}_{\tilde{w}}^2$.
5. Under the identification of TQ with $Q \times \mathfrak{q}$, the tensor h becomes a map from Q to the symmetric bilinear forms on $\mathfrak{q}$. Consequently,

$$\begin{aligned} \nabla_v h(q) w^2 &= \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} h\big(q\exp(\tilde{v}\epsilon)\big)\big(\mathrm{Ad}_{\exp(-\tilde{v}\epsilon/2)}\,\tilde{w}\big)^2 \\ &= \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \big(h\big(q\exp(\tilde{v}\epsilon)\big)w^2\big) + h(q)(\tilde{w}, \mathrm{ad}_{\tilde{w}}\,\tilde{v}). \end{aligned} \tag{44}$$

An important special case is obtained by taking $V = 0$ and g to be a left invariant metric; both g and h then determine constant symmetric bilinear forms on $\mathfrak{q}$, which we denote by the same names. One gets, from Equation (30) and the formulas immediately above, and dropping the tilde,

$$g^\flat A(w) = h\left(w, \mathrm{ad}_w - \left(2 - \frac{f_1}{f_2} - \frac{1}{f_2}\right)\left(-\frac{1}{4}\,\mathrm{ad}_w^2\right)\right). \tag{45}$$

The series expansion for $2 - f_1/f_2 - 1/f_2$ has no constant term and the linear map ad_w is $\tilde{g}$ skew symmetric, so one may replace h in (45) by g. Then

$$A(w) = g^\sharp g\left(w, \mathrm{ad}_w - \left(2 - \frac{f_1}{f_2} - \frac{1}{f_2}\right)\left(-\frac{1}{4}\,\mathrm{ad}_w^2\right)\right),$$

and, begining with the state $tv_1 \in \mathfrak{q}$, the implicit part of the algorithm is the iteration of

$$w = tv_1 + \frac{1}{2}A(w). \tag{46}$$

After the Legendre transform, the dynamics of the system occurs on the cotangent bundle $T^\star Q$, and that dynamics descends, by the quotient map that is left translation to the identity, to the quotient $T^\star Q/Q = \mathfrak{q}^\star$, where it becomes a *Lie-Poisson* system [9][10]. On the tangent bundle side, the dynamics descends to $\mathfrak{q}$, again by left translation, where it is equivalent the the Lie-Poisson dynamics of $\mathfrak{q}^\star$ by the linear isomorphism $g^\flat$. Since our algorithm respects the symmetry of left translation, it too descends to integrate the dynamics on $\mathfrak{q}$. If one is interested merely in the dynamics on the quotient, then one simply discards the part of the algorithm that updates configurations. An efficiency can be realized by noting that

$$\frac{1}{2}A(w) + \frac{1}{2}A(-w) = g^\sharp g(w, \mathrm{ad}_w),$$

and then the explicit part of the algorithm yields the state $tv_2 \in \mathfrak{q}$ given by

$$\begin{aligned} tv_2 &= w + \frac{1}{2}A(-w) \\ &= tv_1 + \frac{1}{2}A(w) + \frac{1}{2}A(-w) \\ &= tv_1 + g^\sharp g(w, \mathrm{ad}_w) \end{aligned} \tag{47}$$

Remarkably, the exponential map of the Lie group needs never to be calculated. Another, equivalent algorithm, but directly integrating the Lie-Poisson system on $\mathfrak{q}^\star$, is obtained by transforming this algorithm on $\mathfrak{q}$ by the linear map $g^\flat$, which amounts to the substitution $\pi = g^\flat w$. Both these equivalent *Lie-Poisson integrators* [9] are summarized in Figure (2).

For a different kind of special case, suppose H is a closed subgroup of G and that Q is the homogeneous space of left cosets G/H. Many common diffeotypes are homogeneous spaces: spheres and projective spaces, for example. One gives G/H a Riemannian structure by imposing that the projection $\pi : G \to G/H$ be an isometric immersion ([5] page 104), and one can identify TQ with $G \times \mathfrak{h}^\perp$, where $\mathfrak{h}$ is the Lie algebra of H, by

$$(g, \tilde{w}) \in G \times \mathfrak{h} \mapsto w = \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \pi\big(g \exp(\tilde{w}t)\big).$$

The natural implication of this is that we identify Q with G in the sense that $g \in Q \equiv G$ means $\pi(g)$. Then we have the following:

1. The exponential mapping of the metric on G/H is $\exp_q w = q \exp \tilde{w}$.
2. While not necessarily a symmetric space, G/H is symmetric in a local sense ([5] page 157), and this is enough to imply that the Riemannian curvature tensor is parallel, which in turn validates the results of of Section (4.3).

Lie-Poisson integrator on $\mathfrak{q}$*:* Given an initial state $tv_1 \in \mathfrak{q}$, find $w \in \mathfrak{q}$ by iterating

$$w = tv_1 + g^\sharp g\left(w, \operatorname{ad}_w - \left(2 - \frac{f_1}{f_2} - \frac{1}{f_2}\right)\left(-\frac{1}{4}\operatorname{ad}_w^2\right)\right).$$

The new state is $tv_2 \in \mathfrak{q}$, where

$$tv_2 = tv_1 + g^\sharp g(w, \operatorname{ad}_w).$$

Lie-Poisson integrator on $\mathfrak{q}^*$*:* Given an initial state $t\pi_1 \in \mathfrak{q}^*$, find $\alpha \in \mathfrak{q}^*$ by iterating

$$\alpha = t\pi_1 + \left(\operatorname{ad}_w - \left(2 - \frac{f_1}{f_2} - \frac{1}{f_2}\right)\left(-\frac{1}{4}\operatorname{ad}_w^2\right)\right)^* \alpha,$$

where $w = g^\sharp \alpha$. The new state is $t\pi_2 \in \mathfrak{q}^*$, where

$$t\pi_2 = t\pi_1 + \operatorname{ad}_w^* \alpha.$$

In either case, if the full integration on Q is required, then configurations in Q are updated after each implicit step by left multiplication by $\exp w$.

Fig. 2. The Lie-Poisson algorithm.

3. Parallel translation along the geodesic $\exp_q tw$ is $\mathbb{P}_{tw} v = \operatorname{Ad}_{\exp(-\tilde{w}t/2)} \tilde{v}$. Again, the parallel translations occuring in the algorithm do not change their arguments.
4. The curvature operator may be calculated from page 105 of [5], and is $R_w = -\operatorname{ad}_{\tilde{w}}^2$.
5. With obvious changes in context, ∇hw^2 can be calculated using Equation (44).

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