DISCRETE AND CONTINUOUS
DYNAMICAL SYSTEMS
Supplement 2009

Website: www.aimSciences.org

pp. **220–229**

NUMERICAL AND GEOMETRIC ASPECTS OF THE NONHOLONOMIC SHAKE AND RATTLE METHODS

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Abstract. Here we discuss a geometric integrator for nonholonomic mechanical systems that preserves the nonholonomic constraints, the discrete nonholonomic momentum map, and is also energy-preserving in some important cases. This method does not require a predefined discretization of the nonholonomic constraints. In Euclidean space, it yields a generalization of the classical SHAKE and RATTLE algorithms to the nonholonomic setting. This article shows that the method is second order convergent.

1. **Introduction.** Nonholonomic mechanical systems are those that are subjected to constraints on the velocities that are not just a consequence of restrictions on the positions. Many systems of interest in engineering, such as wheeled vehicles, are of this kind. We mention here the books [2, 4] as good references on the subject.

Recent works, such as [5, 6, 11, 16], have introduced numerical integrators for nonholonomic systems with very good energy behavior and properties such as the preservation of the discrete nonholonomic momentum map.

Preservation of energy in the autonomous case is an important feature of the continuous system. The authors have proposed in [7] a general geometric construction of a method that exactly preserves energy when the configuration space is a Lie group, the Lagrangian is bi-invariant, and the discrete Lagrangian is left-invariant.

When the configuration manifold is $\mathbb{R}^n$ and the kinetic energy metric is constant, the geometric method mentioned above becomes an extension of the classical SHAKE and RATTLE algorithms [17] for nonholonomic systems. The main goal of this paper is to study some numerical properties of this nonholonomic integrator.

Most existing geometric methods rely on having a discretization of the constraints, that is, replacing the restrictions on the velocities by restrictions on pairs of (nearby) points. We must mention that, in contrast, the method studied here does not require such discretizations to be predefined.

2000 *Mathematics Subject Classification.* 37J60, 37M15, 70F25.

Key words and phrases. RATTLE method, holonomic and nonholonomic systems, variational integrators, energy-momentum integrators.

2. **Description of the nonholonomic dynamics.** Let Q be a n-dimensional differentiable manifold, with local coordinates (q^i), $1 \le i \le n$.

Consider a mechanical Lagrangian system $L\colon TQ \to \mathbb{R}$ defined by $L(v_q) = \frac{1}{2}g(v_q, v_q) - V(q)$, $v_q \in T_qQ$. Here g is a Riemannian metric on Q and V represents a potential function. Assume that the system is subjected to nonholonomic constraints, defined by a regular distribution $\mathcal{D}$ on Q with $\operatorname{corank}\mathcal{D} = m$. Using the metric g, we can define the complementary projectors

$$\mathcal{P}\colon TQ \to \mathcal{D} \hookrightarrow TQ$$
$$\mathcal{Q}\colon TQ \to \mathcal{D}^\perp \hookrightarrow TQ$$

and their duals $\mathcal{P}^*$, $\mathcal{Q}^*$, considered as mappings $T^*Q \to T^*Q$.

Locally the nonholonomic constraints are described by the vanishing of m independent functions

$$\phi^a = \mu_i^a(q) \cdot \dot{q}^i, \quad 1 \le a \le m \ \text{ (the "constraint functions").}$$

Lagrange–D'Alembert's principle prescribes that the nonholonomic equations are

$$\nabla_{\dot{c}(t)}\dot{c}(t) = -\operatorname{grad} V(c(t)) + \lambda(t), \quad \dot{c}(t) \in \mathcal{D}_{c(t)},$$

where ∇ is the Levi–Civita connection associated to g and λ is a section of $\mathcal{D}^\perp$ along c. Here $\mathcal{D}^\perp$ stands for the orthogonal complement of $\mathcal{D}$ with respect to g.

In coordinates, by defining the n^3 functions Γ_{ij}^k (Christoffel symbols for ∇) by

$$\nabla_{\frac{\partial}{\partial q^i}} \frac{\partial}{\partial q^j} = \Gamma_{ij}^k \frac{\partial}{\partial q^k},$$

we may rewrite the nonholonomic equations of motion as

$$\begin{cases} \ddot{q}^k(t) + \Gamma_{ij}^k(c(t))\dot{q}^i(t)\dot{q}^j(t) = -g^{ki}(c(t))\dfrac{\partial V}{\partial q^i} + \lambda_a(t)g^{ki}(c(t))\mu_i^a(c(t)) \\ \mu_i^a(c(t))\dot{q}^i(t) = 0 \end{cases}$$

where $t \mapsto (q^1(t), \dots, q^n(t))$ is the local representative of c and (g^{ij}) is the inverse of the matrix (g_{ij}) of the metric.

We now turn to the Hamiltonian description of the nonholonomic system on the cotangent bundle T^*Q of Q [12]. The canonical coordinates on T^*Q are denoted by (q^i, p_i), and the cotangent bundle projection is $\pi_Q\colon T^*Q \to Q$. In this case, the Legendre transformation $\operatorname{Leg}\colon TQ \to T^*Q$ is

$$(q^i, \dot{q}^i) \mapsto (q^i, p_i = \partial L/\partial \dot{q}^i) = (q^i, g_{ij}\dot{q}^j),$$

The constraint functions on T^*Q become $\Psi^a = \phi^a \circ \operatorname{Leg}^{-1}$, i.e.

$$\Psi^a(q^i, p_i) = \phi^a\left(q^i, \frac{\partial H}{\partial p_i}\right) = \mu_i^a(q)g^{ij}(q)p_j\,,$$

where the Hamiltonian $H\colon T^*Q \to \mathbb{R}$ is locally defined by

$$H(q^i, p_i) = \frac{1}{2}g^{ij}p_ip_j + V(q).$$

The equations of motion for the nonholonomic system on T^*Q can be written as

$$\begin{cases} \dot{q}^i = g^{ij}p_j \\ \dot{p}_i = -\dfrac{\partial H}{\partial q^i} + \lambda_a\mu_i^a, \end{cases}$$

together with the constraint equations $\Psi^a(q, p) = \mu_i^a g^{ij} p_j$.

Now define the regular matrix

$$(\mathcal{C}^{ab}) = \left(\mu_i^a g^{ij} \mu_j^b\right).$$

After time differentiation of the nonholonomic constraints, and substituting the equations of motion, we obtain unique values of the Lagrange multipliers λ_a:

$$\lambda_a = -\mathcal{C}_{ab} X_H(\Psi^b), \tag{1}$$

where X_H is the Hamiltonian vector field corresponding to H and $X_H(\Psi^b)$ denotes the vector field X_H applied to the function Ψ^b as a derivation. Therefore, the nonholonomic equations (without Lagrange multipliers) are equivalently written as

$$\begin{cases} \dot{q}^i = \dfrac{\partial H}{\partial p_i} \\ \dot{p}_i = -\dfrac{\partial H}{\partial q^i} - \Lambda_i \,, \end{cases} \tag{2}$$

for initial conditions (q_0, p_0) verifying the nonholonomic constraints and

$$\Lambda_i = -\mathcal{C}_{ab} X_H(\Psi^b) \mu_i^a.$$

This term represents the constraint force once the Lagrange multipliers have been determined.

If the constraints are holonomic, that is, they are determined by a submanifold N of Q, locally determined by the vanishing of the constraint functions $\phi^a(q) = 0$, then the equations of motion assume the known form

$$\begin{cases} \dot{q}^i = g^{ij} p_j \\ \dot{p}_i = -\dfrac{\partial H}{\partial q^i} + \lambda_a \dfrac{\partial \phi^a}{\partial q^i} \\ \phi^a(q) = 0. \end{cases}$$

Observe that the constraint $\frac{\partial \phi^a}{\partial q^i}(q)\dot{q}^i = 0$ is also preserved along the time evolution.

As a particular case of interest (see Section 4), consider a continuous nonholonomic system determined by the mechanical Lagrangian $L\colon \mathbb{R}^{2n} \to \mathbb{R}$:

$$L(q, \dot{q}) = \frac{1}{2} \dot{q}^T M \dot{q} - V(q)$$

(with M a constant, invertible matrix) and the constraints determined by $\mu(q)\dot{q} = 0$ where $\mu(q)$ is a $m \times n$ matrix with $\operatorname{rank} \mu = m$. The associated Hamiltonian is

$$H(q, p) = \frac{1}{2} p^T M^{-1} p + V(q).$$

Then, Equations (2) are rewritten as

$$\begin{cases} \dot{q} = M^{-1} p \\ \dot{p} = -V_q - \mu^T \lambda \\ \mu(q)\dot{q} = 0, \end{cases} \tag{3}$$

where λ is an $m \times 1$ matrix representing the unknown Lagrange multipliers.

In the holonomic case the equations read

$$\begin{cases} \dot{q} = M^{-1} p \\ \dot{p} = -V_q - G^T \lambda \\ \phi^a(q) = 0, \end{cases}$$

where $G = (\partial\phi^a/\partial q^i)$.

Now, return to Equations (3). We can obtain the actual values of the Lagrange multipliers λ as in Equation (1) to get

$$\lambda = \mathcal{C}^{-1}\left(\mu_q[M^{-1}p, M^{-1}p] - \mu M^{-1}V_q\right) \tag{4}$$

where $\mu_q[M^{-1}p, M^{-1}p]$ denotes the $m\times 1$ matrix $\left(\frac{\partial\mu_i^a}{\partial q^j}(M^{-1})^{jj'}p_{j'}(M^{-1})^{ii'}p_{i'}\right)$ and $\mathcal{C} = \mu M^{-1}\mu^T$. Then the equations of motion for the nonholonomic system are

$$\begin{cases} \dot{q} = M^{-1}p \\ \dot{p} = -V_q - \mu^T\mathcal{C}^{-1}\left(\mu_q[M^{-1}p, M^{-1}p] - \mu M^{-1}V_q\right) \end{cases} \tag{5}$$

with initial condition satisfying $\mu(q)M^{-1}p = 0$.

3. SHAKE and RATTLE for holonomic systems.

The problem of performing a numerical simulation of a mechanical system subjected to holonomic constraints is a topic of actual research. The main difficulties are that the propagation of errors in numerical algorithms for holonomic systems is usually more complicated that in the free case and, moreover, it is necessary to resolve accurately the constraint functions in each step of the proposed algorithm.

Trying to solve the previous difficulties, in 1976 Ryckaert, Ciccotti and Berendsen [17] proposed a numerical algorithm (SHAKE method) for integrating $3n$-cartesian equations for a system of n points with holonomic constraints. The main application is molecular dynamics (polymers or biological compounds) where the atomic distances are introduced as holonomic constraints. Given a Hamiltonian function

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

the SHAKE method is a generalization of the classical Störmer–Verlet method in presence of holonomic constraints:

$$q_{k+1} - 2q_k + q_{k-1} = -h^2M^{-1}\left(V_q(q_k) + G^T(q_k)\lambda_k\right) \tag{6a}$$

$$0 = \phi(q_k). \tag{6b}$$

The paper by Andersen [1] introduced in 1983 a related formulation, the RATTLE method (both SHAKE and RATTLE are algebraically equivalent, see [13]):

$$p_{k+1/2} = p_k - \tfrac{h}{2}\left(V_q(q_k) + G^T(q_k)\lambda_k\right), \tag{7a}$$

$$q_{k+1} = q_k + hM^{-1}p_{k+1/2}, \tag{7b}$$

$$0 = \phi(q_{k+1}), \tag{7c}$$

$$p_{k+1} = p_{k+1/2} - \tfrac{h}{2}\left(V_q(q_{k+1}) + G^T(q_{k+1})\bar{\lambda}_{k+1}\right), \tag{7d}$$

$$0 = G(q_{k+1})M^{-1}p_{k+1}. \tag{7e}$$

Equations (7a), (7b) and (7c) constitute a nonlinear system for the unknowns $p_{k+1/2}$, q_{k+1} and λ_k giving a unique solution for initial values q_k, p_k and fixed step h. The same is true for (7d) and (7e) for unknowns p_{k+1} and $\bar{\lambda}_{k+1}$. Therefore, for initial values $(q_0, p_0) \in \mathcal{M}$, where $\mathcal{M} = \{(q,p) \mid \phi(q) = 0,\ G(q)M^{-1}p = 0\}$, we obtain unique values (q_1, p_1) also in $\mathcal{M}$ and successively.

The SHAKE method is a three-term recursion and this can produce an accumulation of round-off errors. The RATTLE method addresses this problem by providing a one-step reformulation [8].

4. **Nonholonomic version of the RATTLE and SHAKE methods.** Consider a continuous nonholonomic system determined by the mechanical Lagrangian $L\colon \mathbb{R}^{2n} \to \mathbb{R}$:

$$L(q,\dot{q}) = \frac{1}{2}\dot{q}^T M \dot{q} - V(q)$$

(with M a constant, invertible matrix) and the constraints determined by $\mu(q)\dot{q} = 0$ where $\mu(q)$ is a $m \times n$ matrix with rank $\mu = m$.

Consider the following equations as an integrator for the nonholonomic system:

$$q_{k+1} - 2q_k + q_{k-1} = -h^2 M^{-1}\left(V_q(q_k) + \mu^T(q_k)\lambda_k\right) \tag{8a}$$

$$0 = \mu(q_k)\left(\frac{q_{k+1} - q_{k-1}}{2h}\right), \tag{8b}$$

where λ_k are Lagrange multipliers. These equations are a special case of a general geometric construction that we proposed in [7] and review in section 5.

We recognize this set of equations as an obvious extension of the SHAKE method of Equation (6) proposed by [17] to the case of nonholonomic constraints. Equations (8) were mentioned in [16] (see equations (5.3) therein) as a reversible method for nonholonomic systems *not based* on the Discrete Lagrange–D'Alembert principle. While [16] uses a velocity formulation and states that it is not clear how to constrain the initial conditions, our following Hamiltonian approach yields natural constraints (see Remark 1 below).

The momentum is approximated by $p_k = M(q_{k+1} - q_{k-1})/2h$. Denoting $p_{k+1/2} = M(q_{k+1} - q_k)/h$, equations (8a) and (8b) are now rewritten in the form

$$\begin{aligned} p_{k+1/2} &= p_k - \frac{h}{2}\left(V_q(q_k) + \mu^T(q_k)\lambda_k\right), \\ q_{k+1} &= q_k + hM^{-1}p_{k+1/2}, \\ 0 &= \mu(q_k)M^{-1}p_k. \end{aligned}$$

The definition of p_{k+1} requires the knowledge of q_{k+2} and, therefore, it is is natural to apply another step of the algorithm (8a) and (8b) to avoid this difficulty. Then, we obtain the new equations:

$$\begin{aligned} p_{k+1} &= p_{k+1/2} - \frac{h}{2}\left(V_q(q_{k+1}) + \mu^T(q_{k+1})\lambda_{k+1}\right), \\ 0 &= \mu(q_{k+1})M^{-1}p_{k+1}. \end{aligned}$$

The interesting result is that we obtain a natural extension of the RATTLE algorithm for holonomic systems to the case of nonholonomic systems. Unifying the equations above we obtain the following numerical scheme

$$p_{k+1/2} = p_k - \tfrac{h}{2}\left(V_q(q_k) + \mu^T(q_k)\lambda_k\right), \tag{9a}$$

$$q_{k+1} = q_k + hM^{-1}p_{k+1/2}, \tag{9b}$$

$$0 = \mu(q_k)M^{-1}p_k, \tag{9c}$$

$$p_{k+1} = p_{k+1/2} - \tfrac{h}{2}\left(V_q(q_{k+1}) + \mu^T(q_{k+1})\lambda_{k+1}\right), \tag{9d}$$

$$0 = \mu(q_{k+1})M^{-1}p_{k+1}. \tag{9e}$$

These equations allow us to take a triple (q_k, p_k, λ_k) satisfying the constraint equations (9c), compute $p_{k+1/2}$ using (9a) and then q_{k+1} using (9b). Then, equations (9d) and (9e) are used to compute the remaining components of the triple

$(q_{k+1}, p_{k+1}, \lambda_{k+1})$. In the next section we will show (see Theorem 5.1) that, in the case $V = 0$, the numerical method is energy preserving.

Remark 1. From this Hamiltonian point of view, we have shown that the initial conditions for this numerical scheme are constrained in a natural way ((q_0, p_0) with $\mu(q_0)M^{-1}p_0 = 0$), that is, the initial conditions are exactly the same as those for the continuous system. Additionally, we select $\lambda_0 = 0$ (see [7]).

Remark 2. In the particular case where the constraints are integrable, that is, the motion is only defined on a submanifold N of Q, locally described by the vanishing of a family of independent functions $\phi^a(q) = 0$, $1 \leq a \leq m$. Differentiating, we obtain new constraints

$$\frac{\partial \phi^a}{\partial q^i}(q)\dot{q}^i = 0 \tag{10}$$

which are satisfied by the trajectories $(q(t), \dot{q}(t))$ in the continuous problem.

If we directly apply our method to a holonomic system we obtain the preservation of constraints (10) but the computed numerical solution will not usually lie on the constraint submanifold $\phi^a(q) = 0$. For instance, it seems more natural to change (9c) by $\phi^a(q_{k+1}) = 0$, as appears in the classical RATTLE method. Nevertheless, in the case $V = 0$, our method has as an additional feature the preservation of energy (see Theorem 5.1). We could say that the proposed method is specifically designed for nonintegrable constraints.

Now, we analyze the convergence of the method using an adaptation of the proof in [13].

Theorem 4.1. *The nonholonomic RATTLE method is globally second-order convergent.*

Proof. Consider the unconstrained problem

$$\dot{q} = M^{-1}p$$
$$\dot{p} = \phi(q, p)$$

with $\phi\colon \mathbb{R}^{2n} \to \mathbb{R}$ a smooth enough function. These equations can be discretized by

$$q_{k+1} = q_k + hM^{-1}p_{k+1/2}$$
$$p_{k+1/2} = p_{k-1/2} + h\phi\left(q_k, \frac{p_{k-1/2} + p_{k+1/2}}{2}\right)$$

which is a second-order global convergent method, using standard arguments of Taylor expansions.

Therefore, from Equations (5), we deduce the following second-order method for the nonholonomic system:

$$q_{k+1} = q_k + hM^{-1}p_{k+1/2} \tag{11a}$$

$$p_{k+1/2} = p_{k-1/2} - hV_q(q_k) + h\mu^T(q_k)\mathcal{C}^{-1}(q_k)\left(\mu(q_k)M^{-1}V_q(q_k) - \mu_q\left[M^{-1}\frac{p_{k-1/2} + p_{k+1/2}}{2}, M^{-1}\frac{p_{k-1/2} + p_{k+1/2}}{2}\right]\right), \tag{11b}$$

using the notation introduced in Equation (4).

From Equations (9) we see that the nonholonomic RATTLE method assumes the leap-frog form:

$$\begin{aligned} q_{k+1} &= q_k + hM^{-1}p_{k+1/2}, \\ p_{k+1/2} &= p_{k-1/2} - hV_q(q_k) - h\mu^T(q_k)\lambda_k, \\ 0 &= \mu(q_k)M^{-1}\left(\frac{p_{k+1/2}+p_{k-1/2}}{2}\right), \end{aligned}$$

or, after some computations,

$$q_{k+1} = q_k + hM^{-1}p_{k+1/2}, \tag{12a}$$

$$\begin{aligned} p_{k+1/2} = {} & p_{k-1/2} - hV_q(q_k) + h\mu^T(q_k)\mathcal{C}^{-1}(q_k)\mu(q_k)M^{-1}V_q(q_k) \\ & - 2\mu^T(q_k)\mathcal{C}^{-1}(q_k)\mu(q_k)M^{-1}p_{k-1/2}. \end{aligned} \tag{12b}$$

Now, expanding the nonholonomic constraints around $q = q(0)$ and evaluating at $q = q(h)$ we obtain:

$$\mu(q(h))\dot{q}(h) = \mu(q(0))\dot{q}(0) + h\left(\mu(q(0))\ddot{q}(0) + \mu_q[\dot{q}(0),\dot{q}(0)]\right) + O(h^2).$$

Therefore,

$$h\mu(q(0))\ddot{q}(0) = -h\mu_q[\dot{q}(0),\dot{q}(0)] + O(h^2).$$

Now, taking standard approximations we deduce that

$$\begin{aligned} &\mu(q_k)M^{-1}\left(p_{k+1/2} - p_{k-1/2}\right) \\ &\quad = -h\mu_q\left[M^{-1}\frac{p_{k-1/2}+p_{k+1/2}}{2}, M^{-1}\frac{p_{k-1/2}+p_{k+1/2}}{2}\right] + O(h^2), \end{aligned} \tag{13}$$

where now $q(0) = q_k$, $q(h) = q_{k+1}$, etc.

From the constraint equations we have that:

$$\mu(q_k)M^{-1}\left(\frac{p_{k+1/2}+p_{k-1/2}}{2}\right) = O(h^2) \tag{14}$$

Therefore, from (13) and (14), we deduce

$$\begin{aligned} &-2\mu(q_k)M^{-1}p_{k-1/2} \\ &\quad = -h\mu_q\left[M^{-1}\frac{p_{k-1/2}+p_{k+1/2}}{2}, M^{-1}\frac{p_{k-1/2}+p_{k+1/2}}{2}\right] + O(h^2). \end{aligned} \tag{15}$$

Substituting expression (15) in (12b) we recognize Equation (11b). Since the nonholonomic RATTLE method is obviously symmetric, we deduce that is globally second-order convergent. □

5. **On the geometric construction of nonholonomic integrators.** The nonholonomic RATTLE method is a special case of a wider category of numerical methods (see [7]). The construction is strongly based on the use of the discrete variational principle to obtain the discrete Euler–Lagrange equations for *unconstrained* systems ([15]):

$$D_1L_d(q_k,q_{k+1}) + D_2L_d(q_{k-1},q_k) = 0.$$

where $L_d\colon Q\times Q\to\mathbb{R}$ is a discretization of the continuous Lagrangian $L\colon TQ\to\mathbb{R}$.

The ***discrete nonholonomic equations*** proposed in [7] are

$$\mathcal{P}^*_{|q_k}(D_1L_d(q_k,q_{k+1})) + \mathcal{P}^*_{|q_k}(D_2L_d(q_{k-1},q_k)) = 0 \tag{16a}$$

$$\mathcal{Q}^*_{|q_k}(D_1L_d(q_k,q_{k+1})) - \mathcal{Q}^*_{|q_k}(D_2L_d(q_{k-1},q_k)) = 0. \tag{16b}$$

The first equation is the projection of the discrete Euler–Lagrange equations to the dual of the constraint distribution $\mathcal{D}$, while the second one can be interpreted as an elastic impact of the system against $\mathcal{D}$ (see [10]).

This defines a unique discrete evolution operator if and only if the matrix $(D_{12}L_d)$ is regular, i.e., if the discrete Lagrangian is regular. From these equations, the covector $D_1L_d(q_k,q_{k+1}) + D_2L_d(q_{k-1},q_k)$ annihilates $\mathcal{D}$, while the vector obtained from $D_1L_d(q_k,q_{k+1}) - D_2L_d(q_{k-1},q_k)$ by index raising with the metric lies in $\mathcal{D}$. Locally, if the nonholonomic constraints are given by $\mu^a_i(q)\dot{q}^i = 0$, $1 \le a \le m$, where m is the corank of $\mathcal{D}$, then these equations can be written as

$$D_1L_d(q_k,q_{k+1}) + D_2L_d(q_{k-1},q_k) = (\lambda_k)_b\,\mu^b$$

$$g^{ij}(q_k)\mu^a_i(q_k)\left(\frac{\partial L_d}{\partial q^j_0}(q_k,q_{k+1}) - \frac{\partial L_d}{\partial q^j_1}(q_{k-1},q_k)\right) = 0.$$

Observe that equations (8), and hence the nonholonomic RATTLE method, appears when taking the symmetric discretization

$$\begin{aligned} L_d(q_k,q_{k+1}) &= \frac{1}{2}hL\left(q_k, \frac{q_{k+1}-q_k}{h}\right) + \frac{1}{2}hL\left(q_{k+1}, \frac{q_{k+1}-q_k}{h}\right) \\ &= \frac{1}{2h}\left(q_{k+1}-q_k\right)^T M\left(q_{k+1}-q_k\right) - \frac{h}{2}\left(V(q_k)+V(q_{k+1})\right) \end{aligned}$$

for the continuous Lagrangian

$$L(q,\dot{q}) = \frac{1}{2}\dot{q}^T M\dot{q} - V(q)\,.$$

Define the pre- and post-momenta using the discrete Legendre transformations:

$$p^+_{k-1,k} = \mathbb{F}^+L_d(q_{k-1},q_k) = (q_k, D_2L_d(q_{k-1},q_k)) \in T^*_{q_k}Q$$

$$p^-_{k,k+1} = \mathbb{F}^-L_d(q_k,q_{k+1}) = (q_k, -D_1L_d(q_k,q_{k+1})) \in T^*_{q_k}Q.$$

In these terms, equation (16b) can be rewritten as

$$\mathcal{Q}^*_{|q_k}\left(\frac{p^-_{k,k+1}+p^+_{k-1,k}}{2}\right) = 0$$

which means that the average of post- and pre-momenta satisfies the constraints. We can also rewrite the discrete nonholonomic equations as a jump of momenta:

$$p^-_{k,k+1} = (\mathcal{P}^* - \mathcal{Q}^*)\,\big|_{q_k}(p^+_{k-1,k}).$$

5.1. **Left-invariant systems on Lie groups.** Take $Q = G$ a Lie group, with elements denoted as γ_k, and a left-invariant discrete Lagrangian ([3, 14]). Define the increment $W_k = \gamma_k^{-1}\gamma_{k+1}$. By computing the derivatives involved in Equations (16) and using the invariance of the discrete Lagrangian (see [7] for details), the method becomes

$$p^-_{k,k+1} = (\mathcal{P} - \mathcal{Q})^*\left(R^*_{W^{-1}_{k-1}}\,p^-_{k-1,k}\right) \tag{17}$$

where R^* is the mapping on T^*G induced by right multiplication. The method is illustrated in the terms of this equation in Figure 1.

If in addition $\mathcal{D}$ is left-invariant, then

$$p_k = (\mathcal{P} - \mathcal{Q})^* \left(\mathrm{Ad}^*_{W_{k-1}} p_{k-1} \right),$$

where p_k is the discrete body momentum ([6]) $p_k = L^*_{\gamma_k} p^-_{k,k+1} \in \mathfrak{g}^*$.

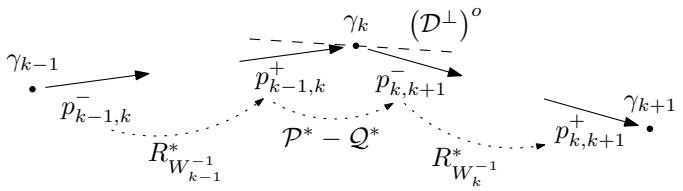

FIGURE 1. Evolution of momenta (solid arrows) according to Eq. (17).

5.2. **Preservation of energy and momentum.** The preservation of energy, momentum and/or symplectic form, are important geometric properties for an integrator to have, if the continuous system also preserves these quantities. It is well-known [9] that it is not possible to construct an integrator that is energy, momentum, and symplectic preserving, unless it is the exact integrator. The method that we study here is energy and momentum preserving. In any case, since the continuous nonholonomic evolution is not symplectic, it makes little sense to try to obtain a symplectic nonholonomic integrator. The following theorem is proven in [7], and we show here a sketch of the proof for completeness.

Theorem 5.1. *Let the configuration manifold be a Lie group with a bi-invariant Lagrangian and with an arbitrary distribution $\mathcal{D}$, and take a discrete Lagrangian that is left-invariant. Then the discrete nonholonomic method (16) is energy-preserving.*

Sketch of proof. The bi-invariant metric g induces a bi-invariant inner product on each fiber of T^*G. Right translations on T^*G and the mapping $(\mathcal{P} - \mathcal{Q})^* \colon T^*G \to T^*G$ preserve the corresponding norm $\| \cdot \|_g$. Then the method (17) is such that $\|p^-_{k,k+1}\|_g$ (and also $\|p^+_{k,k+1}\|_g$) is preserved. The potential energy must be zero, so the energy is the Hamiltonian $H = \frac{1}{2}\|p\|^2_g$, which is therefore preserved. □

Note that if the Lagrangian L is bi-invariant, then it is possible to take a particular discretization scheme that makes the discrete Lagrangian L_d bi-invariant [14]. Nevertheless, it is sufficient to have a left-invariant L_d for the theorem to hold, since it relies on equation (17).

The example of the snakeboard [7] has an interesting feature: the Lagrangian is not bi-invariant at first, but this can be circumvented by changing the group structure of the configuration manifold $\mathrm{SE}(2) \times \mathrm{S}^2$ into an abelian one. The method is not altered, and the preservation of energy follows.

Suppose that Q is a manifold on which a Lie group G acts. Define for each $q \in Q$

$$\mathfrak{g}^q = \{ \xi \in \mathfrak{g} \,|\, \xi_Q(q) \in \mathcal{D}_q \},$$

where $\xi_Q(q)$ is the infinitesimal generator vector field corresponding to $\xi \in \mathfrak{g}$ at the point q. The bundle over Q whose fiber at q is $\mathfrak{g}^q$ is denoted by $\mathfrak{g}^{\mathcal{D}}$. Define the discrete nonholonomic momentum map $J^{\mathrm{nh}}_d \colon Q \times Q \to (\mathfrak{g}^{\mathcal{D}})^*$ as in [5] by

$$\begin{aligned} J^{\mathrm{nh}}_d(q_{k-1}, q_k) \colon \mathfrak{g}^{q_k} &\to \mathbb{R} \\ \xi &\mapsto \langle D_2 L_d(q_{k-1}, q_k), \xi_Q(q_k) \rangle . \end{aligned}$$

For any smooth section $\widetilde{\xi}$ of $\mathfrak{g}^{\mathcal{P}}$ we have a function $(J_d^{\mathrm{nh}})_{\widetilde{\xi}}\colon Q \times Q \to \mathbb{R}$, defined as $(J_d^{\mathrm{nh}})_{\widetilde{\xi}}(q_{k-1}, q_k) = J_d^{\mathrm{nh}}(q_{k-1}, q_k)\left(\widetilde{\xi}(q_k)\right)$.

If L_d is G-invariant and $\xi \in \mathfrak{g}$ is a horizontal symmetry (that is, $\xi_Q(q) \in \mathcal{D}_q$ for all $q \in Q$), then this nonholonomic integrator preserves $(J_d^{\mathrm{nh}})_{\xi}$ (see [7] for a proof).

Acknowledgments. This work has been partially supported by MEC (Spain) Grant MTM 2007-62478, project "Ingenio Mathematica" (i-MATH) No. CSD 2006-00032 (Consolider-Ingenio 2010) and Project SIMUMAT S-0505/ESP/0158 of the CAM. S. Ferraro thanks SIMUMAT for a research contract and Centre Interfacultaire Bernoulli for a research stay. D. Iglesias thanks CSIC for a JAE Research Contract. The authors wish to thank Miguel A. López Marcos for helpful comments and the referees, who suggested important improvements upon the first version of our paper.

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Received August 2008; revised April 2009.

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