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New developments on the geometric nonholonomic integrator

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Abstract

In this paper, we will discuss new developments regarding the geometric nonholonomic integrator (GNI) (Ferraro *et al* 2008 *Nonlinearity* **21** 1911–28; Ferraro *et al* 2009 *Discrete Contin. Dyn. Syst.* (Suppl.) 220–9). GNI is a discretization scheme adapted to nonholonomic mechanical systems through a discrete geometric approach. This method was designed to account for some of the special geometric structures associated to a nonholonomic motion, like preservation of energy, preservation of constraints or the nonholonomic momentum equation. First, we study the GNI versions of the symplectic-Euler methods, paying special attention to their convergence behaviour. Then, we construct an extension of the GNI in the case of affine constraints. Finally, we generalize the proposed method to nonholonomic reduced systems, an important subclass of examples in nonholonomic dynamics. We illustrate the behaviour of the proposed method with the example of the inhomogeneous sphere rolling without slipping on a table.

Keywords: geometric nonholonomic integrator, nonholonomic mechanics, discrete variational calculus, reduction by symmetries, affine constraints
Mathematics Subject Classification: 70F25, 37J60, 37M15, 37N05, 65P10, 70-08

1. Introduction

Nonholonomic constraints have been a subject of deep analysis since the dawn of analytical mechanics. The origin of its study is nicely explained in the introduction of the book by Neimark and Fufaev [47],

> The birth of the theory of dynamics of nonholonomic systems occurred at the time when the universal and brilliant analytical formalism created by Euler and Lagrange was found, to general amazement, to be inapplicable to the very simple mechanical problems of rigid bodies rolling without slipping on a plane. Lindelöf's error, detected by Chaplygin, became famous and rolling systems attracted the attention of many eminent scientists of the time...

Many authors have recently shown a new interest in that theory and also in its relationship to the new developments in control theory and robotics. The main characteristic of this last period is that nonholonomic systems are studied from a geometric perspective (see [54] as an advanced and fundamental reference, and also, [3,5,6,14,17,34,36,39] and references therein). From this perspective, nonholonomic mechanics forms part of a wider body of research called *geometric mechanics*.

A nonholonomic system is a mechanical system subjected to constraint functions which are, roughly speaking, functions on the velocities that are not derivable from position constraints. They arise, for instance, in mechanical systems that have rolling or certain kinds of sliding contact. Traditionally, the equations of motion for nonholonomic mechanics are derived from the Lagrange–d'Alembert principle, which restricts the set of infinitesimal variations (or constrained forces) in terms of the constraint functions. In such systems, some differences between unconstrained classical Hamiltonian and Lagrangian systems and nonholonomic dynamics appear. For instance, nonholonomic systems are non-variational in the classical sense, since they arise from the Lagrange–d'Alembert principle and not from Hamilton's principle. Moreover, when the nonholonomic constraints are linear in velocities and a symmetry arises, energy is preserved but in general momentum is not. Nonholonomic systems are described by an almost-Poisson structure (i.e. there is a bracket that together with the energy on the phase space defines the motion, but the bracket generally does not satisfy the Jacobi identity); and finally, unlike the Hamiltonian setting, volume may not be preserved in the phase space, leading to interesting asymptotic stability in some cases, despite energy conservation which is a consequence of the homogeneity in velocities of the constraints.

From the applied point of view, in the last decade great interest has been focused on the study of the dynamical behaviour of some particular examples of nonholonomic systems; more concretely, different rigid bodies rolling without slipping (either with or without spinning) of on a plane or on a sphere. Besides, a hierarchy has been constructed in terms of the body's surface geometry and mass distribution.

The existence of an invariant measure and Hamiltonization of such systems, and the necessary conditions for this existence have been carefully studied in [9–11, 35]. See [3, 5, 14, 17, 34, 39, 54] for more details about nonholonomic systems.

Recent works, firstly initiated by J Cortés and S Martínez in their seminal paper [19], where the authors introduce the notion of discrete Lagrange–d'Alembert's principle, have been devoted to derive numerical methods for nonholonomic systems (see [21, 28, 41, 31]). These numerical integrators for nonholonomic systems have very good energy behaviour in simulations and additional properties such as the preservation of the discrete nonholonomic momentum map. In a different direction, some of the authors of this paper have introduced the geometric nonholonomic integrator (GNI), whose properties and original motivations can be found in [23], while some of its applications and numerical performance can be found in [24, 32]. Particularly, in [32] we have examined numerically the GNI and the reduced d'Alembert–Pontryagin integrator (RDP) in some typical examples of nonholonomic mechanics: the Chaplygin sleigh and the snakeboard. In a different approach, numerical schemes based on the Hamiltonization of nonholonomic systems have been explored in [22,45]. Although these methods have shown an excellent qualitative and quantitative behaviour, they are quite difficult to implement with generality since they involve solving a difficult task: the Hamiltonization or an inverse problem for a nonholonomic system [4].

Our aim in this work is to analyse further developments of the GNI method introduced in the mentioned references. Particularly, we focus on two aspects: the GNI extension of the usual symplectic-Euler methods (we prove their consistency order and the fact that they are the adjoint of one another), and the generalization of the method to new situations, namely the cases of affine constraints (definition 6.1), reduction by a Lie group of symmetries (definition 7.1) and Lie algebroids (definition 8.2). All the new generalizations are appropriately illustrated with theoretical and numerical results.

The paper is structured as follows: section 2 is devoted to introduce the continuous nonholonomic problem with linear constraints, to obtain the nonholonomic equations by means of the Lagrange–d'Alembert principle and to show how these equations can be reobtained through a projection procedure when the system is endowed with a Riemannian metric. Section 3 summarizes the general theory of variational integrators, while section 4 presents the proposed GNI. In section 5, the GNI versions of the symplectic-Euler methods are obtained and their convergence behaviour studied in theorem 5.2. It is also proved in theorem 5.4 that both methods are adjoint of each other; this fact establishes an interesting parallelism with the free (meaning *unconstrained*) variational integrators. Section 6 accounts for the affine extension of the GNI which is illustrated with the theoretical result of SHAKE and RATTLE methods. Section 7 is devoted to the development of the GNI for reduced systems, in the case of both linear and affine constraints. The former case is illustrated with the theoretical result of RATTLE algorithm while the latter (which is also affine) is carefully treated in the example of the Chaplygin sphere with three different moments of inertia, including some numerical results. Finally, in section 8 we extend the GNI to Lie algebroids.

2. Continuous nonholonomic mechanics

Mathematically, the nonholonomic setting can be described as follows. We shall start with a configuration space Q, which is an n-dimensional differentiable manifold with local coordinates denoted by q^i, $i = 1, \ldots, n = \dim Q$, and a non-integrable distribution $\mathcal{D}$ on Q that describes the linear nonholonomic constraints. We can consider this constant-rank distribution $\mathcal{D}$ as a vector subbundle of the tangent bundle TQ (velocity phase space) of the configuration space. Moreover, and as we mentioned in the introduction, $\mathcal{D}$ defines a set of constraints on the velocities. Locally, the linear constraints are written as follows:

$$\phi^a(q, \dot{q}) = \mu_i^a(q)\, \dot{q}^i = 0, \qquad 1 \leqslant a \leqslant m, \tag{1}$$

where $\operatorname{rank}(\mathcal{D}) = n - m$. The annihilator $\mathcal{D}^\circ$ is locally given by

$$\mathcal{D}^\circ = \operatorname{span}\left\{\mu^a = \mu_i^a(q)\, \mathrm{d}q^i; \qquad 1 \leqslant a \leqslant m\right\},$$

where the 1-forms μ^a are independent.

In addition to the distribution, we need to specify the dynamical evolution of the system, usually by fixing a Lagrangian function $L : TQ \to \mathbb{R}$. In nonholonomic mechanics, the procedure permitting the extension from the Newtonian point of view to the Lagrangian one is given by the Lagrange–d'Alembert principle. This principle states that a curve $q : I \subset \mathbb{R} \to Q$ is an admissible motion of the system if

$$\delta \mathcal{J} = \delta \int_0^T L\left(q\left(t\right), \dot{q}\left(t\right)\right) \mathrm{d}t = 0$$

for all variations such that $\delta q(t) \in \mathcal{D}_{q(t)}$, $0 \leqslant t \leqslant T$, and if the velocity of the curve itself satisfies the constraints. It is remarkable that the Lagrange–d'Alembert principle is not variational since we are imposing the constraints on the curve 'after extremizing' the functional $\mathcal{J}$. From Lagrange–d'Alembert's principle, we arrive to the nonholonomic equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}^i}\right) - \frac{\partial L}{\partial q^i} = \lambda_a \mu_i^a, \tag{2a}$$

$$\mu_i^a(q)\,\dot{q}^i = 0, \tag{2b}$$

where $\lambda_a,\ a = 1, \ldots, m$ is a set of Lagrange multipliers. The right-hand side of equation (2*a*) represents the force induced by the constraints, and equations (2*b*) represent the constraints themselves.

Now we are going to restrict ourselves to the case of nonholonomic mechanical systems with mechanical Lagrangian, i.e.

$$L\left(v_q\right) = \frac{1}{2}\mathcal{G}\left(v_q, v_q\right) - V\left(q\right), \quad v_q \in T_q Q, \tag{3}$$

where $\mathcal{G}$ is a Riemannian metric on the configuration space Q locally determined by the matrix $M = (\mathcal{G}_{ij})_{1\leqslant i,j\leqslant n}$, where $\mathcal{G}_{ij} = \mathcal{G}(\partial/\partial q^i, \partial/\partial q^j)$. Using some basic tools of Riemannian geometry (see, for instance, [13]), we may write the equations of motion of the unconstrained system determined by L as

$$\nabla_{\dot{c}(t)}\dot{c}\left(t\right) = -\mathrm{grad}\, V\left(c\left(t\right)\right), \tag{4}$$

where ∇ is the Levi–Civita connection associated with $\mathcal{G}$. Observe that if $V \equiv 0$ then the Euler–Lagrange equations become the geodesic equations for the Levi–Civita connection.

When the system is subjected to nonholonomic constraints, the equations turn out to be

$$\nabla_{\dot{c}(t)}\dot{c}\left(t\right) = -\mathrm{grad}\, V\left(c\left(t\right)\right) + \lambda\left(c\left(t\right)\right), \qquad \dot{c}\left(t\right) \in \mathcal{D}_{c(t)},$$

where λ is a section of $\mathcal{D}^\perp$ along c (see [3, 13, 14]). Here, $\mathcal{D}^\perp$ stands for the orthogonal complement of $\mathcal{D}$ with respect to $\mathcal{G}$.

Since Q is equipped with a Riemannian metric, we can decompose the tangent bundle as $TQ = \mathcal{D} \oplus \mathcal{D}^\perp$. Moreover, we can also construct two complementary projectors $\mathcal{P} : TQ \to \mathcal{D}$, $\mathcal{Q} : TQ \to \mathcal{D}^\perp$. In order to obtain a local expression for $\mathcal{P}$ and $\mathcal{Q}$, define the vector fields Z^a, $1 \leqslant a \leqslant m$, on Q by

$$\mathcal{G}\left(Z^a, Y\right) = \mu^a\left(Y\right), \quad \text{for all } Y \in \mathfrak{X}(M),$$

that is, Z^a is the gradient vector field of the 1-form μ^a. Thus, $\mathcal{D}^\perp$ is spanned by Z^a, $1 \leqslant a \leqslant m$. In local coordinates:

$$Z^a = \mathcal{G}^{ij}\mu_i^a \frac{\partial}{\partial q^j}.$$

Considering the $m \times m$ matrix $(C^{ab}) = (\mu_i^a\, \mathcal{G}^{ij}\, \mu_j^b)$ (which is symmetric and regular since $\mathcal{G}$ is a Riemannian metric), we obtain the local description of $\mathcal{Q}$:

$$\mathcal{Q} = C_{ab} Z^a \otimes \mu^b = C_{ab}\mathcal{G}^{ij}\mu_i^a \mu_k^b \frac{\partial}{\partial q^j} \otimes \mathrm{d}q^k,$$

and $\mathcal{P} = \mathrm{Id}_{TQ} - \mathcal{Q}$. Finally, by using these projectors we may rewrite the equation of motion as follows. A curve $c(t)$ is a motion of the nonholonomic system if it satisfies the constraints, i.e. $\dot{c}(t) \in \mathcal{D}_{c(t)}$, and, in addition, the 'projected equation of motion'

$$\mathcal{P}\left(\nabla_{\dot{c}(t)}\dot{c}\,(t)\right) = -\mathcal{P}\,(\mathrm{grad}\,V\,(c\,(t))) \tag{5}$$

is fulfilled.

Summarizing, we have obtained the dynamics of the nonholonomic system (5) applying the projector $\mathcal{P}$ to the unconstrained equations of motion (4).

3. Discrete mechanics and variational integrators

Variational integrators are a kind of geometric integrators for the Euler–Lagrange equations which retain their variational character and also, as a consequence, some of main geometric properties of the continuous system, such as symplecticity and momentum conservation (see [25, 43, 46, 55]). In the following we will summarize the main features of this type of geometric integrators. A *discrete Lagrangian* is a map $L_d : Q \times Q \to \mathbb{R}$, which may be considered as an approximation of the action integral defined by a continuous Lagrangian $L: TQ \to \mathbb{R}$, that is, $L_d(q_0, q_1) \approx \int_0^h L(q(t), \dot{q}(t))\,\mathrm{d}t$, where $q(t)$ is a solution of the Euler–Lagrange equations for L joining $q(0) = q_0$ and $q(h) = q_1$ for small enough $h > 0$.

Define the *action sum* $S_d: Q^{N+1} \to \mathbb{R}$ corresponding to the Lagrangian L_d by $S_d = \sum_{k=1}^{N} L_d(q_{k-1}, q_k)$, where $q_k \in Q$ for $0 \leqslant k \leqslant N$, where N is the number of steps. The discrete variational principle states that the solutions of the discrete system determined by L_d must extremize the action sum given fixed endpoints q_0 and q_N. By extremizing S_d over q_k, $1 \leqslant k \leqslant N-1$, we obtain the system of difference equations

$$D_1 L_d(q_k, q_{k+1}) + D_2 L_d(q_{k-1}, q_k) = 0. \tag{6}$$

These equations are usually called the *discrete Euler–Lagrange equations*. Under some regularity hypotheses (the matrix $(D_{12}L_d(q_k, q_{k+1}))$ is regular), it is possible to define from (6) a (local) discrete flow $\Upsilon_{L_d}: Q \times Q \to Q \times Q$, by $\Upsilon_{L_d}(q_{k-1}, q_k) = (q_k, q_{k+1})$. Define the discrete Legendre transformations associated to L_d as

$$\begin{aligned}
\mathbb{F}L_d^-: Q \times Q &\to T^*Q\\
(q_k, q_{k+1}) &\longmapsto (q_k, -D_1 L_d(q_k, q_{k+1})),\\
\mathbb{F}L_d^+: Q \times Q &\to T^*Q\\
(q_k, q_{k+1}) &\longmapsto (q_{k+1}, D_2 L_d(q_k, q_{k+1})),
\end{aligned}$$

and the discrete Poincaré–Cartan 2-form $\omega_d = (\mathbb{F}L_d^+)^*\omega_Q = (\mathbb{F}L_d^-)^*\omega_Q$, where ω_Q is the canonical symplectic form on T^*Q. The discrete algorithm determined by Υ_{L_d} preserves the symplectic form ω_d, i.e. $\Upsilon_{L_d}^*\omega_d = \omega_d$. Moreover, if the discrete Lagrangian is invariant under the diagonal action of a Lie group G, then the discrete momentum map $J_d: Q \times Q \to \mathfrak{g}^*$ defined by

$$\langle J_d(q_k, q_{k+1}), \xi\rangle = \langle D_2 L_d(q_k, q_{k+1}), \xi_Q(q_{k+1})\rangle$$

is preserved by the discrete flow. Therefore, these integrators are symplectic-momentum preserving. Here, ξ_Q denotes the fundamental vector field determined by $\xi \in \mathfrak{g}$, where $\mathfrak{g}$ is the Lie algebra of G. (See [43] for more details.)

4. The geometric nonholonomic integrator

The geometric nonholonomic integrator (GNI in the sequel) and its principal features have been presented in [23, 24, 33]. As main geometric properties, we can mention that it preserves the nonholonomic constraints, the discrete nonholonomic momentum map in the presence of horizontal symmetries, and the energy of the system under certain symmetry conditions [23].

Definition 4.1. *Consider a discrete Lagrangian* $L_d : Q \times Q \to \mathbb{R}$*. The proposed* discrete nonholonomic equations *are*

$$\mathcal{P}^*_{q_k}\left(D_1 L_d\left(q_k, q_{k+1}\right)\right) + \mathcal{P}^*_{q_k}\left(D_2 L_d\left(q_{k-1}, q_k\right)\right) = 0, \tag{7a}$$

$$\mathcal{Q}^*_{q_k}\left(D_1 L_d\left(q_k, q_{k+1}\right)\right) - \mathcal{Q}^*_{q_k}\left(D_2 L_d\left(q_{k-1}, q_k\right)\right) = 0, \tag{7b}$$

which define the GNI

The projectors $\mathcal{P}$, $\mathcal{Q}$ are defined in the previous sections, while the subscript q_k emphasizes that the projections take place in the fibre $T^*_{q_k}Q$. The first equation is just the projection of the discrete Euler–Lagrange equation to the constraint distribution $\mathcal{D}$, while the second one can be interpreted as an elastic impact of the system against $\mathcal{D}$ (see [27]). Note that since $\mathcal{P}$ and $\mathcal{Q}$ are orthogonal and complementary, (7) is equivalent to

$$D_1 L_d(q_k, q_{k+1}) + (\mathcal{P}^* - \mathcal{Q}^*)\, D_2 L_d(q_{k-1}, q_k) = 0. \tag{8}$$

From these equations we see that the system defines a unique discrete evolution operator if and only if the matrix $(D_{12} L_d)$ is regular, that is, the discrete Lagrangian is regular. Locally, equations (7) can be written as

$$D_1 L_d\left(q_k, q_{k+1}\right) + D_2 L_d\left(q_{k-1}, q_k\right) = (\lambda_k)_b\, \mu^b(q_k), \tag{9a}$$

$$\mathcal{G}^{ij}\left(q_k\right) \mu^a_i\left(q_k\right) \left(\frac{\partial L_d}{\partial x^j}\left(q_k, q_{k+1}\right) - \frac{\partial L_d}{\partial y^j}\left(q_{k-1}, q_k\right)\right) = 0. \tag{9b}$$

Using the discrete Legendre transformations defined above, let us define the pre- and post-momenta, which are covectors at q_k, by

$$p^+_{k-1,k} = p^+\left(q_{k-1}, q_k\right) = \mathbb{F}L^+_d\left(q_{k-1}, q_k\right) = D_2 L_d\left(q_{k-1}, q_k\right)$$

$$p^-_{k,k+1} = p^-\left(q_k, q_{k+1}\right) = \mathbb{F}L^-_d\left(q_k, q_{k+1}\right) = -D_1 L_d\left(q_k, q_{k+1}\right).$$

Then, the second GNI equation (9*b*) can be rewritten as follows:

$$\mathcal{G}^{ij}\left(q_k\right) \mu^a_i\left(q_k\right) \left(\frac{(p^-_{k,k+1})_j + (p^+_{k-1,k})_j}{2}\right) = 0,$$

which means that the average of pre- and post-momenta satisfies the constraints. In this sense the proposed numerical method preserves exactly the nonholonomic constraints. Besides this preservation property, the GNI has other interesting geometric features like the preservation of energy when the configuration manifold is a Lie group with a Lagrangian defined by a bi-invariant metric, with an arbitrary distribution $\mathcal{D}$ and a discrete Lagrangian that is left-invariant (see [23] for further details).

5. GNI extensions of symplectic-Euler methods

Let us consider the tangent TQ and cotangent T^*Q bundles of the configuration manifold $Q = \mathbb{R}^n$ and its local coordinates, $(q, \dot{q})$ and (q, p) respectively. Moreover, let us consider the mechanical Lagrangian $L(q, \dot{q}) = \frac{1}{2}\dot{q}^T M \dot{q} - V(q)$, where M is a $n \times n$ constant regular matrix and $V : Q \to \mathbb{R}$ is the potential function. On the other hand, the function $H(q, p) = \frac{1}{2} p^T M^{-1} p + V(q)$ is its Hamiltonian counterpart.

It is well known that the explicit and implicit Euler methods (which we will denote Euler A and Euler B respectively)

$$\begin{array}{cc} \text{Euler A} & \text{Euler B} \\ q_{k+1} = q_k + hM^{-1} p_k & q_{k+1} = q_k + hM^{-1} p_{k+1} \\ p_{k+1} = p_k - h\dfrac{\partial V}{\partial q}(q_k) & p_{k+1} = p_k - h\dfrac{\partial V}{\partial q}(q_{k+1}) \end{array}$$

are symplectic and of order one (see [25]). As variational integrators (see [43]) they correspond to the following discrete Lagrangians:

$$L_d^A(q_k, q_{k+1}) = hL\left(q_k, \frac{q_{k+1} - q_k}{h}\right), \quad L_d^B(q_k, q_{k+1}) = hL\left(q_{k+1}, \frac{q_{k+1} - q_k}{h}\right). \tag{10}$$

Applying the GNI equations (9) to the Lagrangians in (10) we obtain the following numerical schemes:

- **Euler A**:

$$q_{k+1} - 2q_k + q_{k-1} = -h^2 M^{-1}\left(V_q(q_k) + \mu^T(q_k)\,\tilde{\lambda}_k\right), \tag{11a}$$

$$0 = \mu(q_k)\left(\frac{q_{k+1} - q_{k-1}}{2h} + \frac{h}{2}M^{-1}V_q(q_k)\right). \tag{11b}$$

- **Euler B**:

$$q_{k+1} - 2q_k + q_{k-1} = -h^2 M^{-1}\left(V_q(q_k) + \mu^T(q_k)\,\tilde{\lambda}_k\right), \tag{12a}$$

$$0 = \mu(q_k)\left(\frac{q_{k+1} - q_{k-1}}{2h} - \frac{h}{2}M^{-1}V_q(q_k)\right), \tag{12b}$$

where $\tilde{\lambda}_k = \lambda_k/h$ and $V_q = \partial V/\partial q$. Observe that the only difference between the two methods lies in the sign between parentheses in (11b) and (12b). By introducing the momentum quantities $\tilde{p}_k = M(q_{k+1} - q_{k-1})/2h$ and $p_{k+1/2} = M(q_{k+1} - q_k)/h$, we can rewrite equations (11) and (12) as follows.

- **Euler A**:

$$p_{k+1/2} = \tilde{p}_k - \frac{h}{2}\left(V_q(q_k) + \mu^T(q_k)\tilde{\lambda}_k\right), \tag{13a}$$

$$q_{k+1} = q_k + hM^{-1}p_{k+1/2}, \tag{13b}$$

$$\mu(q_k)M^{-1}\left(\tilde{p}_k + \frac{h}{2}V_q(q_k)\right) = 0, \tag{13c}$$

$$\tilde{p}_{k+1} = p_{k+1/2} - \frac{h}{2}\left(V_q(q_{k+1}) + \mu^T(q_{k+1})\tilde{\lambda}_{k+1}\right), \tag{13d}$$

$$\mu(q_{k+1})M^{-1}\left(\tilde{p}_{k+1} + \frac{h}{2}V_q(q_{k+1})\right) = 0. \tag{13e}$$

- **Euler B**:

$$p_{k+1/2} = \tilde{p}_k - \frac{h}{2}\left(V_q(q_k) + \mu^T(q_k)\tilde{\lambda}_k\right), \tag{14a}$$

$$q_{k+1} = q_k + hM^{-1}p_{k+1/2}, \tag{14b}$$

$$\mu(q_k)M^{-1}\left(\tilde{p}_k - \frac{h}{2}V_q(q_k)\right) = 0, \tag{14c}$$

$$\tilde{p}_{k+1} = p_{k+1/2} - \frac{h}{2}\left(V_q(q_{k+1}) + \mu^T(q_{k+1})\tilde{\lambda}_{k+1}\right), \tag{14d}$$

$$\mu(q_{k+1})M^{-1}\left(\tilde{p}_{k+1} - \frac{h}{2}V_q(q_{k+1})\right) = 0. \tag{14e}$$

These numerical schemes provide values at step $k+1$ through an intermediate momentum step $k + 1/2$, i.e.

$$(q_k, \tilde{p}_k, \tilde{\lambda}_k) \to (q_{k+1}, p_{k+1/2}, \tilde{\lambda}_k) \to (q_{k+1}, \tilde{p}_{k+1}, \tilde{\lambda}_{k+1}).$$

We recognize in (13*c*), (13*e*) and (14*c*), (14*e*) a Hamiltonian version for the discretization of the nonholonomic constraints (11*b*) and (12*b*) (Lagrangian version). These constraints are provided by the GNI equations (7*b*) or (9*b*).

Remark 5.1. Method (11) (and the corresponding B version) clearly resembles the extension of the SHAKE method (see [50]) proposed by McLachlan and Perlmutter [41] as a reversible method for nonholonomic systems *not based* on the discrete Lagrange–d'Alembert principle, namely

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

At the same time, the SHAKE method is an extension of the classical Störmer–Verlet method in the presence of holonomic constraints. The RATTLE method is algebraically equivalent to SHAKE [37]. Its nonholonomic extension, introduced for the first time in [41], that is

$$p_{k+1/2} = \tilde{p}_k - \frac{h}{2}\left(V_q(q_k) + \mu^T(q_k)\tilde{\lambda}_k\right), \tag{15a}$$

$$q_{k+1} = q_k + hM^{-1}p_{k+1/2}, \tag{15b}$$

$$\mu(q_k)M^{-1}\tilde{p}_k = 0, \tag{15c}$$

$$\tilde{p}_{k+1} = p_{k+1/2} - \frac{h}{2}\left(V_q(q_{k+1}) + \mu^T(q_{k+1})\tilde{\lambda}_{k+1}\right), \tag{15d}$$

$$\mu(q_{k+1})M^{-1}\tilde{p}_{k+1} = 0 \tag{15e}$$

(see [23]) clearly resembles (13).

As shown in [23], the nonholonomic SHAKE extension can be obtained by applying the GNI equations to the discrete Lagrangian

$$L_d(q_k, q_{k+1}) = \frac{h}{2}L\left(q_k, \frac{q_{k+1} - q_k}{h}\right) + \frac{h}{2}L\left(q_{k+1}, \frac{q_{k+1} - q_k}{h}\right), \tag{16}$$

which also provides the Störmer–Verlet method in the variational integrators sense. Moreover, as shown in [24], the nonholonomic RATTLE method (15) is globally second-order convergent.

Theorem 5.2. *The nonholonomic extension of the Euler A (B) method is globally first-order convergent.*

It will be useful in the following proof to give a Hamiltonian version of (2) when $H(q, p) = \frac{1}{2}p^T M^{-1} p + V(q)$, namely

$$\begin{aligned} \dot{q} &= M^{-1}p, \\ \dot{p} &= -V_q(q) - \mu^T(q)\lambda, \\ \mu(q)\, M^{-1}p &= 0. \end{aligned}$$

Since the constraints are satisfied along the solutions, we can differentiate them w.r.t. time in order to obtain the actual values of the Lagrange multipliers, i.e.

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

where $\mathcal{C}(q) = \mu(q)M^{-1}\mu^T(q)$ is a regular matrix and $\mu_q[M^{-1}p, M^{-1}p]$ is the $m \times 1$ matrix $\frac{\partial \mu_i^\alpha}{\partial q^j}(M^{-1})^{jj'}p_{j'}(M^{-1})^{ii'}p_{i'}$. Taking this into account, the Hamiltonian nonholonomic system becomes

$$\dot{q} = M^{-1}p, \tag{17a}$$
$$\dot{p} = -V_q - \mu^T\mathcal{C}^{-1}\left(\mu_q[M^{-1}p, M^{-1}p] - \mu M^{-1}V_q\right), \tag{17b}$$

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

Proof of theorem 5.2. We present the proof for the Euler A method, the corresponding proof for Euler B is analogous.

Consider the unconstrained problem

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

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

$$q_{k+1} = q_k + hM^{-1}p_{k+1/2}, \tag{18a}$$
$$p_{k+1/2} = p_{k-1/2} + h\phi\left(q_k, p_{k+1/2}\right), \tag{18b}$$

which is a globally first-order convergent method, using standard arguments of Taylor expansions. Therefore, taking into account equations (17), from (18) we deduce the following first-order method for the nonholonomic system

$$q_{k+1} = q_k + hM^{-1}p_{k+1/2}, \tag{19a}$$
$$\begin{aligned} p_{k+1/2} = p_{k-1/2} &- hV_q(q_k) + h\mu^T(q_k)\,\mathcal{C}^{-1}(q_k)\,\mu(q_k)\,M^{-1}V_q(q_k) \\ &- h\mu^T(q_k)\,\mathcal{C}^{-1}(q_k)\,\mu_q[M^{-1}p_{k+1/2}, M^{-1}p_{k+1/2}]. \end{aligned} \tag{19b}$$

The next step is to prove that the nonholonomic Euler A method (13) reproduces (19). From equations (13) we see that the nonholonomic Euler A method assumes the form

$$q_{k+1} = q_k + hM^{-1}p_{k+1/2},$$
$$p_{k+1/2} = p_{k-1/2} - hV_q(q_k) - h\mu^T(q_k)\tilde{\lambda}_k,$$
$$0 = \mu(q_k)M^{-1}\left(\frac{p_{k+1/2} + p_{k-1/2}}{2} + \frac{h}{2}V_q(q_k)\right)$$

or, after some computations,

$$q_{k+1} = q_k + hM^{-1}p_{k+1/2}, \tag{20a}$$
$$p_{k+1/2} = p_{k-1/2} - hV_q(q_k) - 2\mu^T(q_k)\mathcal{C}^{-1}(q_k)\mu(q_k)M^{-1}p_{k-1/2}. \tag{20b}$$

On the other hand we can expand the nonholonomic constraints around $q(0)$:

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

Since the constraints are satisfied at $t = 0$ and $t = h$, the previous expression becomes

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

Now, taking standard approximations for first and second derivatives we deduce that

$$\begin{aligned} -2\mu(q_k)M^{-1}p_{k-1/2} = &-h\mu_q[M^{-1}p_{k+1/2}, M^{-1}p_{k+1/2}] \\ &+h\mu(q_k)M^{-1}V_q(q_k) + \mathcal{O}(h^2). \end{aligned} \tag{21}$$

Therefore, substituting (21) into (20*b*) we recognize equation (19*b*) up to $\mathcal{O}(h^2)$ terms. Thus, we conclude that the nonholonomic Euler A method (13) is first-order convergent. □

Definition 5.3. *For a one-step method $F : T^*Q \to T^*Q$, the adjoint method $F^* : T^*Q \to T^*Q$ is defined by*

$$(F^*)^h \circ F^{-h} = Id_{T^*Q}.$$

Theorem 5.4. *The nonholonomic extensions of the Euler A and B methods are one another's adjoint.*

Proof. We will use a shorthand notation to define both integrators:

$$F_A(q_k, \tilde{p}_k, \tilde{\lambda}_k) = (q^A_{k+1}, \tilde{p}^A_{k+1}, \tilde{\lambda}^A_{k+1}),$$
$$F_B(q_k, \tilde{p}_k, \tilde{\lambda}_k) = (q^B_{k+1}, \tilde{p}^B_{k+1}, \tilde{\lambda}^B_{k+1}).$$

Equations (13) and (14) can be rewritten to give a one-step method instead of the leap-frog presented. For instance, for F_A,

$$q^A_{k+1} = q_k + hM^{-1}\tilde{p}_k - \frac{h^2}{2}M^{-1}V_q(q_k) - \frac{h^2}{2}M^{-1}\mu^T(q_k)\tilde{\lambda}_k, \qquad (22a)$$

$$\tilde{p}^A_{k+1} = \tilde{p}_k - \frac{h}{2}V_q(q_k) - \frac{h}{2}\mu^T(q_k)\tilde{\lambda}_k - \frac{h}{2}V_q(q^A_{k+1}) - \frac{h}{2}\mu^T(q^A_{k+1})\tilde{\lambda}^A_{k+1}, \qquad (22b)$$

$$0 = \mu(q^A_{k+1})M^{-1}\tilde{p}_k - \frac{h}{2}\mu(q^A_{k+1})M^{-1}V_q(q_k) - \frac{h}{2}\mu(q^A_{k+1})M^{-1}\mu^T(q_k)\tilde{\lambda}_k$$
$$-\frac{h}{2}\mu(q^A_{k+1})M^{-1}\mu^T(q^A_{k+1})\tilde{\lambda}^A_{k+1}, \qquad (22c)$$

where $\tilde{p}^A_{k+1}$ and $\tilde{\lambda}^A_{k+1}$ are implicitly obtained from (22*b*) and (22*c*). The same occurs for F_B:

$$q^B_{k+1} = q_k + hM^{-1}\tilde{p}_k - \frac{h^2}{2}M^{-1}V_q(q_k) - \frac{h^2}{2}M^{-1}\mu^T(q_k)\tilde{\lambda}_k, \qquad (23a)$$

$$\tilde{p}^B_{k+1} = \tilde{p}_k - \frac{h}{2}V_q(q_k) - \frac{h}{2}\mu^T(q_k)\tilde{\lambda}_k - \frac{h}{2}V_q(q^B_{k+1}) - \frac{h}{2}\mu^T(q^B_{k+1})\tilde{\lambda}^B_{k+1}, \qquad (23b)$$

$$0 = -\mu(q_k)M^{-1}\tilde{p}^B_{k+1} - \frac{h}{2}\mu(q_k)M^{-1}V_q(q^B_{k+1}) - \frac{h}{2}\mu(q_k)M^{-1}\mu^T(q_k)\tilde{\lambda}_k$$
$$-\frac{h}{2}\mu(q_k)M^{-1}\mu^T(q^B_{k+1})\tilde{\lambda}^B_{k+1}. \qquad (23c)$$

The point of the proof is to show that $F^h_A \circ F^{-h}_B(q_k, \tilde{p}_k, \tilde{\lambda}_k) = (q_k, \tilde{p}_k, \tilde{\lambda}_k)$. In order to do that, we are going to use the notation

$$F^{-h}_B(q_k, \tilde{p}_k, \tilde{\lambda}_k) = (q_{k+1}, \tilde{p}_{k+1}, \tilde{\lambda}_{k+1}) = (q'_k, \tilde{p}'_k, \tilde{\lambda}'_k),$$
$$F^h_A(q'_k, \tilde{p}'_k, \tilde{\lambda}'_k) = (q'_{k+1}, \tilde{p}'_{k+1}, \tilde{\lambda}'_{k+1}),$$

so we need to show that $(q'_{k+1}, \tilde{p}'_{k+1}, \tilde{\lambda}'_{k+1}) = (q_k, \tilde{p}_k, \tilde{\lambda}_k)$. After setting the time step to $-h$ and replacing (23*a*) and (23*b*) into (22*a*), it is easy to check that $q'_{k+1} = q_k$. Furthermore, fixing $-h$ again as the time step and taking into account equation (14*e*), from (23*c*) we arrive to

$$-\frac{h}{2}M^{-1}\mu^T(q'_k)\tilde{\lambda}'_k = -M^{-1}\tilde{p}_k - \frac{h}{2}V_q(q_k) - M^{-1}\tilde{p}'_k + \frac{h}{2}V_q(q'_k) + \frac{h}{2}M^{-1}\mu^T(q_k)\tilde{\lambda}_k.$$

Replacing this expression into (22*c*), considering that $q'_{k+1} = q_k$ and taking into account (13*e*) we find that

$$\frac{h}{2}\mu(q_k)M^{-1}\mu^T(q_k)\tilde{\lambda}_k - \frac{h}{2}\mu(q_k)M^{-1}\mu^T(q_k)\tilde{\lambda}'_{k+1} = 0,$$

which means

$$\tilde{\lambda}'_{k+1} = \tilde{\lambda}_k$$

since $\mathcal{C}(q_k)$ is regular. Finally, replacing (23*b*) into (22*b*) we find that $\tilde{p}'_{k+1} = \tilde{p}_k$. □

Remark 5.5. As shown in [43], the composition of Hamiltonian discrete flows, in the *variational integrators* sense, generated by the discrete Lagrangians (10) reproduces the RATTLE algorithm in the free case (that is, not constrained). More concretely, the composition

$$F_{L_A}^{h/2} \circ F_{L_B}^{h/2}$$

produces the algorithm

$$\begin{aligned} p_{k+1/2} &= \tilde{p}_k - \frac{h}{2} V_q(q_k), \\ q_{k+1} &= q_k + hM^{-1} p_{k+1/2}, \\ \tilde{p}_{k+1} &= p_{k+1/2} - \frac{h}{2} V_q(q_{k+1}). \end{aligned}$$

Unfortunately, this is no longer true in the nonholonomic case, i.e. one can check that the composition (with time step $h/2$) of methods (13) and (14) does not reproduce the equations presented in remark 5.1. However, this composition still generates a second order method since the intermediate steps are first-order methods which are each other's adjoint (as we have just proved).

6. Affine extension of the GNI

We consider in this section the case of affine nonholonomic constraints determined by an affine subbundle $\mathcal{A}$ of TQ modelled on a vector subbundle $\mathcal{D}$. We will assume, in the sequel, that there exists a globally defined vector field $Y \in \mathfrak{X}(Q)$ such that $v_q \in \mathcal{A}_q$ if and only if $v_q - Y(q) \in \mathcal{D}_q$. Therefore, if $\mathcal{D}$ is determined by constraints $\mu_i^a(q)\dot{q}^i = 0$, then $\mathcal{A}$ is locally determined by the vanishing of the constraints

$$\phi^a(q, \dot{q}) = \mu_i^a(q)\left(\dot{q}^i - Y^i(q)\right) = 0, \qquad 1 \leqslant a \leqslant m, \tag{24}$$

where $Y = Y^i \frac{\partial}{\partial q^i}$.

In consequence, the initial data defining our *nonholonomic affine system* is denoted by the 4-tuple $(\mathcal{D}, \mathcal{G}, Y, V)$, where $\mathcal{D}$ is the distribution, $\mathcal{G}$ the Riemannian metric, Y the globally defined vector field and V the potential function. By means of the metric, from Y, we can uniquely define a 1-form $\mathcal{G}(Y, \cdot) = \Pi \in \Omega^1(Q)$. Locally, $\Pi = \mathcal{G}_{ij} Y^j \, \mathrm{d}q^i$.

In terms of momenta the nonholonomic constraints (24) can be rewritten as

$$\mu_i^a(q)\, \mathcal{G}^{ij}\left(p_j - \Pi_j(q)\right) = 0, \tag{25}$$

where $p_i = \mathcal{G}_{ij}\dot{q}^j$.

Definition 6.1. *Consider a discrete Lagrangian* $L_d : Q \times Q \to \mathbb{R}$. *The proposed discrete equations for affine nonholonomic constraints are*

$$\mathcal{P}_{q_k}^*\left(D_1 L_d(q_k, q_{k+1})\right) + \mathcal{P}_{q_k}^*\left(D_2 L_d(q_{k-1}, q_k)\right) = 0, \tag{26a}$$
$$\mathcal{Q}_{q_k}^*\left(D_1 L_d(q_k, q_{k+1})\right) - \mathcal{Q}_{q_k}^*\left(D_2 L_d(q_{k-1}, q_k)\right) + 2\mathcal{Q}_{q_k}^*\Pi = 0, \tag{26b}$$

which define the affine extension of the GNI method.

As before, $\mathcal{Q}$ and $\mathcal{P}$ are the projectors defined in section 2. Locally, the method (26) can be written as

$$D_1 L_d(q_k, q_{k+1}) + D_2 L_d(q_{k-1}, q_k) = (\lambda_k)_b\, \mu^b(q_k), \tag{27a}$$
$$\mathcal{G}^{ij}(q_k)\mu_i^a(q_k)\left(\frac{\partial L_d}{\partial x^j}(q_k, q_{k+1}) - \frac{\partial L_d}{\partial y^j}(q_{k-1}, q_k) + 2\Pi_j(q_k)\right) = 0. \tag{27b}$$

Using the pre- and post-momenta defined in section 4, equation (27*b*) can be rewritten as

$$\mathcal{G}^{ij}(q_k)\mu_i^a(q_k)\left(\frac{\left(p^-_{k,k+1}\right)_j+\left(p^+_{k-1,k}\right)_j}{2}-\Pi_j(q_k)\right)=0,$$

which corresponds to the discretization of the affine constraints (25) on the Hamiltonian side.

6.1. A theoretical result: nonholonomic SHAKE and RATTLE extensions for affine systems

Let us consider again the mechanical Lagrangian $L(q,\dot q)=\frac{1}{2}\dot q^T M\dot q-V(q)$ and the discretization presented in (16). Applying the affine GNI equations (27) we obtain

$$q_{k+1}-2q_k+q_{k-1}=-h^2M^{-1}\left(V_q(q_k)+\mu^T(q_k)\,\tilde\lambda_k\right),\tag{28a}$$

$$0=\mu(q_k)\left(\frac{q_{k+1}-q_{k-1}}{2h}-Y(q_k)\right),\tag{28b}$$

which can be regarded as the extension of the SHAKE algorithm to affine nonholonomic systems. Denoting $\tilde p_k=M(q_{k+1}-q_{k-1})/2h$ and $p_{k+1/2}=M(q_{k+1}-q_k)/h$, from (28) we arrive to

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

which can be regarded as the extension of the RATTLE algorithm to affine nonholonomic systems.

7. Reduced systems

In this section we are going to consider configuration spaces of the form $Q=M\times G$, where M is an n-dimensional differentiable manifold and G is an m-dimensional Lie group ($\mathfrak{g}$ will be its corresponding Lie algebra). Therefore, there exists a global canonical splitting between variables describing the position and variables describing the orientation of the mechanical system. Then, we distinguish the pose coordinates $g\in G$, and the variables describing the internal shape of the system, that is $x\in M$ (in consequence $(x,\dot x)\in TM$). It is clear that $Q=M\times G$ is the total space of a trivial principal G-bundle over M, where the bundle projection $\phi:Q\to M$ is just the canonical projection onto the first factor. We may consider the corresponding reduced tangent space $E=TQ/G$ over M. Identifying TG with $G\times\mathfrak{g}$ by using left translations, $E=TQ/G$ is isomorphic to the product manifold $TM\times\mathfrak{g}$ and the vector bundle projection is $\tau_M\circ pr_1$, where $pr_1:TM\times\mathfrak{g}\to TM$ and $\tau_M:TM\to M$ are the canonical projections.

7.1. The case of linear constraints

Now suppose that $(\mathcal{G},\mathcal{D},V)$ is a standard mechanical nonholonomic system on TQ such that all the ingredients are G-invariant. In other words, for all $x\in M$ and $g\in G$,

- $\mathcal{G}_{(x,g)}((X_x,g\xi),(Y_x,g\eta))=\mathcal{G}_{(x,e)}((X_x,\xi),(Y_x,\eta))$ for all $X_x,Y_x\in T_xM$, $\xi,\eta\in\mathfrak{g}$;

- $(X_x, \xi) \in \mathcal{D}_{(x,e)}$ implies $(X_x, g\xi) \in \mathcal{D}_{(x,g)}$;
- $V(x, g) = V(x, e) \equiv \tilde{V}(x)$.

Therefore, we obtain a new triple $(\tilde{\mathcal{G}}, \widetilde{\mathcal{D}}, \tilde{V})$ on $TM \times \mathfrak{g}$ where $\tilde{\mathcal{G}} : (TM \times \mathfrak{g}) \times (TM \times \mathfrak{g}) \longrightarrow \mathbb{R}$ is a bundle metric, $\widetilde{\mathcal{D}}$ is a vector subbundle of $TM \times \mathfrak{g} \to M$ and $\tilde{V} : M \to \mathbb{R}$ is the reduced potential. With all these ingredients it is possible to write the reduced nonholonomic equations or *nonholonomic Lagrange–Poincaré equations* (see [5, 18] for all the details, also for the non-trivial case).

Our objective is to find a discrete version of the GNI for the nonholonomic Lagrange–Poincaré equations. As in the previous sections, we can split the total space E as $E = \widetilde{\mathcal{D}} \oplus \widetilde{\mathcal{D}}^{\perp}$, using this time the fibred metric $\tilde{\mathcal{G}}$, and consider the corresponding projectors $\mathcal{P} : E \to \widetilde{\mathcal{D}}$, $\mathcal{Q} : E \to \widetilde{\mathcal{D}}^{\perp}$. In order to write the discrete nonholonomic equations, it is necessary to set a discrete Lagrangian $L_d : M \times M \times G \to \mathbb{R}$, and the discrete Legendre transforms. Namely (see [44]):

$$\begin{aligned}
&\mathbb{F}L_d^{-}\colon M \times M \times G \to T^*M \times \mathfrak{g}^*\\
&(x_k, x_{k+1}, g_k) \longmapsto (x_k, -D_1L_d(x_k, x_{k+1}, g_k), r^*_{g_k} D_3L_d(x_k, x_{k+1}, g_k)),\\
&\mathbb{F}L_d^{+}\colon M \times M \times G \to T^*M \times \mathfrak{g}^*\\
&(x_k, x_{k+1}, g_k) \longmapsto (x_{k+1}, D_2L_d(x_k, x_{k+1}, g_k), l^*_{g_k} D_3L_d(x_k, x_{k+1}, g_k)) .
\end{aligned} \tag{29}$$

Definition 7.1. Consider the discrete Legendre transforms defined in (29). The proposed discrete equations are

$$\mathcal{P}^*_{x_k}\left(\mathbb{F}L_d^{-}(x_k, x_{k+1}, g_k)\right) - \mathcal{P}^*_{x_k}\left(\mathbb{F}L_d^{+}(x_{k-1}, x_k, g_{k-1})\right) = 0, \tag{30a}$$

$$\mathcal{Q}^*_{x_k}\left(\mathbb{F}L_d^{-}(x_k, x_{k+1}, g_k)\right) + \mathcal{Q}^*_{x_k}\left(\mathbb{F}L_d^{+}(x_{k-1}, x_k, g_{k-1})\right) = 0, \tag{30b}$$

which define the reduced GNI equations. The subscript x_k emphasizes the fact that the projections take place in the fibre over x_k.

To understand why (30*b*) represents a discretization of the nonholonomic constraints, we will work in local coordinates. Take now local coordinates (x^i) on M and a local basis of sections $\{\tilde{e}_\alpha, \tilde{e}_a\}$ of $\Gamma(TM \times \mathfrak{g})$ adapted to the decomposition $\widetilde{\mathcal{D}} \oplus \widetilde{\mathcal{D}}^{\perp}$, that is $\tilde{e}_\alpha(x) \in \widetilde{\mathcal{D}}_x$ and $\tilde{e}_a(x) \in \widetilde{\mathcal{D}}^{\perp}_x$, for all $x \in M$. We have that

$$\tilde{\mathcal{G}}(\tilde{e}_\alpha, \tilde{e}_\beta) = \tilde{\mathcal{G}}_{\alpha\beta}, \quad \tilde{\mathcal{G}}(\tilde{e}_a, \tilde{e}_\beta) = 0, \quad \tilde{\mathcal{G}}(\tilde{e}_a, \tilde{e}_b) = \tilde{\mathcal{G}}_{ab} .$$

Consider the induced adapted local coordinates (x^i, y^α, y^a) for $\Gamma(TM \times \mathfrak{g})$. The nonholonomic constraints are represented by $y^a = 0$ on E. Taking the dual basis $\{\tilde{e}^\alpha, \tilde{e}^a\}$ of $\Gamma(T^*M \times \mathfrak{g}^*)$, we have induced local coordinates (x^i, p_α, p_a) on the Hamiltonian side, and now the nonholonomic constraints are represented by $p_a = 0$.

On the other hand, in this basis the projector $\mathcal{Q}$ has the expression

$$\mathcal{Q} = \tilde{e}^a \otimes \tilde{e}_a. \tag{31}$$

Define the pre- and post-momenta by

$$\begin{aligned}
p^-_{x_k} &= \mathbb{F}L_d^{-}(x_k, x_{k+1}, g_k) \in T^*_{x_k}M \times \mathfrak{g}^*,\\
p^+_{x_k} &= \mathbb{F}L_d^{+}(x_{k-1}, x_k, g_{k-1}) \in T^*_{x_k}M \times \mathfrak{g}^*.
\end{aligned}$$

From equation (30*b*) we obtain

$$\mathcal{Q}^*_{x_k}\left(\frac{p^+_{x_k} + p^-_{x_k}}{2}\right) = 0. \tag{32}$$

If $p^+_{x_k} = p^+_\alpha e^\alpha(x_k) + p^+_a e^a(x_k)$ and $p^-_{x_k} = p^-_\alpha e^\alpha(x_k) + p^-_a e^a(x_k)$, then condition (32) is expressed using (31) as

$$\frac{p^+_a + p^-_a}{2} = 0,$$

which means that the average of post and pre-momenta satisfies the nonholonomic constraints written on the Hamiltonian side.

7.2. A theoretical result: RATTLE algorithm for reduced spaces

Let us consider $M = \mathbb{R}^n$. Thus, $Q = \mathbb{R}^n \times G$ and $E = TQ/G \cong T\mathbb{R}^n \times \mathfrak{g}$. Take a basis $\{E_s\}$ of the Lie algebra $\mathfrak{g}$, and consider the following global basis of $\Gamma(T\mathbb{R}^n \times \mathfrak{g})$

$$\left\{ \left(\frac{\partial}{\partial x^i}, 0 \right), (0, E_s) \right\}.$$

Therefore, its dual basis is

$$\left\{ \left(\mathrm{d}x^i, 0\right), \left(0, E^s\right) \right\}.$$

Writing $\mathrm{d}x^i \equiv (\mathrm{d}x^i, 0)$ and $E^s \equiv (0, E^s)$ for short, the bundle metric $\tilde{\mathcal{G}}$ is written in this basis of sections as

$$\tilde{\mathcal{G}} = \tilde{\mathcal{G}}_{ij}\, \mathrm{d}x^i \otimes \mathrm{d}x^j + \tilde{\mathcal{G}}_{it}\, \mathrm{d}x^i \otimes E^t + \tilde{\mathcal{G}}_{sj} E^s \otimes \mathrm{d}x^j + \tilde{\mathcal{G}}_{st} E^s \otimes E^t.$$

Assume that, in this expression, the coefficients of the bundle metric are symmetric and constant, that is, they do not depend on the base coordinates x. For instance, a typical example would be the kinetic energy bundle metric corresponding to the Lagrangian

$$L(x, \dot{x}, \xi) = \frac{1}{2}\dot{x}^T M \dot{x} + \frac{1}{2}\langle \xi, \mathbb{I}\xi \rangle,$$

where M is a regular symmetric matrix and $\mathbb{I} : \mathfrak{g} \to \mathfrak{g}^*$ is a symmetric positive definite inertia operator.

Consider the discrete Lagrangian $L_d : \mathbb{R}^n \times \mathbb{R}^n \times G \to \mathbb{R}$ defined by

$$L_d(x_k, x_{k+1}, g_k) = \frac{h}{2}\tilde{\mathcal{G}}_{ij} \left(\frac{x^i_{k+1} - x^i_k}{h} \right) \left(\frac{x^j_{k+1} - x^j_k}{h} \right) + h\tilde{\mathcal{G}}_{it} \left(\frac{x^i_{k+1} - x^i_k}{h} \right) \frac{\left(\tau^{-1}(g_k)\right)^t}{h}$$
$$+ \frac{h}{2}\tilde{\mathcal{G}}_{st} \frac{\left(\tau^{-1}(g_k)\right)^s}{h} \frac{\left(\tau^{-1}(g_k)\right)^t}{h} - \frac{h}{2}\left(V(x_k) + V(x_{k+1})\right),$$

where $\tau : \mathfrak{g} \to G$ is a *retraction map*, which is an analytic local diffeomorphism which maps a neighbourhood of $0 \in \mathfrak{g}$ onto a neighbourhood of the neutral element $e \in G$ (see the appendix). Observe that $\tau^{-1}(g_k) \in \mathfrak{g}$ and $\tau^{-1}(g_k) = (\tau^{-1}(g_k))^s E_s$.

Additionally, we have the vector subbundle $\mathfrak{D}$ of $T\mathbb{R}^n \times \mathfrak{g}$ prescribing the nonholonomic constraints. Write $\widetilde{\mathfrak{D}}^\circ = \mathrm{span}\{\mu^a_i dx^i + \eta^a_s E^s\}$. Equation (30*a*) of the GNI method is clearly equivalent to

$$\mathbb{F}L^-_d(x_k, x_{k+1}, g_k) - \mathbb{F}L^+_d(x_{k-1}, x_k, g_{k-1}) \in \widetilde{\mathfrak{D}}^\circ(x_k),$$

which in this case splits into

$$\frac{1}{h}\tilde{\mathcal{G}}_{ij}(x^j_{k+1} - 2x^j_k + x^j_{k-1}) + \frac{1}{h}\tilde{\mathcal{G}}_{it}\left((\tau^{-1}(g_k))^t - (\tau^{-1}(g_{k-1})^t)\right)$$
$$+hV_{x^i}(x_k) = -\lambda_{a,k}\, \mu^a_i(x_k), \tag{33a}$$

$$\ell^*_{g_{k-1}} D_3 L_d(x_{k-1}, x_k, g_{k-1}) - r^*_{g_k} D_3 L_d(x_k, x_{k+1}, g_k) = \lambda_{a,k}\, \eta^a_s(x_k)\, E^s, \tag{33b}$$

where V_{x^i} stands for $\partial V/\partial x^i$, and $\lambda_{a,k}$ are the Lagrange multipliers which might vary in each step.

Equation (33*b*) can be rewritten taking into account the *right trivialized tangent retraction map* $\mathrm{d}\tau_\xi$ for $\xi \in \mathfrak{g}$, defined as

$$\mathrm{d}\tau_\xi = T_{\tau(\xi)} r_{\tau(\xi)^{-1}} \circ T_\xi \tau \colon \mathfrak{g} \to \mathfrak{g}, \tag{34}$$

where $T_\xi\tau\colon\ T_\xi\mathfrak{g} \equiv \mathfrak{g} \to T_{\tau(\xi)}G$, and its inverse $\mathrm{d}\tau_\xi^{-1}$ (see also definition 9.1).

Define the *retracted discrete Lagrangian* $l_d\colon \mathbb{R}^n \times \mathbb{R}^n \times \mathfrak{g} \to \mathbb{R}$ as $l_d(x_k, x_{k+1}, \sigma_k) = L_d(x_k, x_{k+1}, \tau(\sigma_k))$. For example, for the discrete Lagrangian L_d defined above,

$$l_d(x_k, x_{k+1}, \sigma_k) = \frac{h}{2}\tilde{\mathbb{G}}_{ij}\left(\frac{x^i_{k+1} - x^i_k}{h}\right)\left(\frac{x^j_{k+1} - x^j_k}{h}\right) + h\tilde{\mathbb{G}}_{it}\left(\frac{x^i_{k+1} - x^i_k}{h}\right)\frac{\sigma^t_k}{h}$$
$$+\frac{h}{2}\tilde{\mathbb{G}}_{st}\frac{\sigma^s_k}{h}\frac{\sigma^t_k}{h} - \frac{h}{2}\left(V(x_k) + V(x_{k+1})\right).$$

Note that σ_k/h plays the role of a velocity in the Lie algebra direction, so σ_k represents a small change in the pose variables after time h. In this sense, σ_k is analogous to the pair (x_k, x_{k+1}). One has

$$D_3 l_d(x_k, x_{k+1}, \sigma_k) = D_3 L_d(x_k, x_{k+1}, \tau(\sigma_k)) \circ T_{\sigma_k}\tau.$$

Using lemma 9.5 and definition 9.1 in the appendix, one can compute

$$\begin{aligned}(\mathrm{d}\tau^{-1}_{-\sigma_k})^* D_3 l_d(x_k, x_{k+1}, \sigma_k) &= D_3 L_d(x_k, x_{k+1}, \tau(\sigma_k)) \circ T_{\sigma_k}\tau \circ \mathrm{d}\tau^{-1}_{-\sigma_k} = \\ &= D_3 L_d(x_k, x_{k+1}, \tau(\sigma_k)) \circ T_{\sigma_k}\tau \circ \mathrm{d}\tau^{-1}_{\sigma_k} \circ \mathrm{Ad}_{\tau(\sigma_k)} = \\ &= D_3 L_d(x_k, x_{k+1}, \tau(\sigma_k)) \circ T_{\sigma_k}\tau \circ (T_{\sigma_k}\tau)^{-1} \circ T_e r_{\tau(\sigma_k)} \circ \mathrm{Ad}_{\tau(\sigma_k)} = \\ &= D_3 L_d(x_k, x_{k+1}, \tau(\sigma_k)) \circ T_e \ell_{\tau(\sigma_k)}\end{aligned}$$

and

$$\begin{aligned}(\mathrm{d}\tau^{-1}_{\sigma_k})^* D_3 l_d(x_k, x_{k+1}, \sigma_k) &= D_3 L_d(x_k, x_{k+1}, \tau(\sigma_k)) \circ T_{\sigma_k}\tau \circ \mathrm{d}\tau^{-1}_{\sigma_k} = \\ &= D_3 L_d(x_k, x_{k+1}, \tau(\sigma_k)) \circ T_{\sigma_k}\tau \circ (T_{\sigma_k}\tau)^{-1} \circ T_e r_{\tau(\sigma_k)} \\ &= D_3 L_d(x_k, x_{k+1}, \tau(\sigma_k)) \circ T_e r_{\tau(\sigma_k)}.\end{aligned}$$

Therefore, setting $g_k = \tau(\sigma_k)$ and $\sigma_k = h\xi_k$, equation (33*b*) becomes

$$\begin{aligned}&(\mathrm{d}\tau^{-1}_{-h\xi_{k-1}})^* D_3 l_d(x_{k-1}, x_k, h\xi_{k-1}) - (\mathrm{d}\tau^{-1}_{h\xi_k})^* D_3 l_d(x_k, x_{k+1}, h\xi_k) \\ &\quad = \lambda_{a,k}\,\eta^a_t(x_k)\,E^t.\end{aligned} \tag{35}$$

Generally speaking, in most applications one could bypass the definition of L_d and choose l_d to be defined by

$$l_d(x_k, x_{k+1}, \sigma_k) = hL\left(\frac{x_k + x_{k+1}}{2}, \frac{x_{k+1} - x_k}{h}, \frac{\sigma_k}{h}\right)$$

or a similar formula.

As we know, (30*b*) provides a discretization of the nonholonomic constraints on the Hamiltonian side:

$$\begin{aligned}&A^{i,a}(x_k)\left(\tilde{\mathbb{G}}_{ij}\frac{(x^j_{k+1} - x^j_{k-1})}{2h} + \frac{1}{2h}\tilde{\mathbb{G}}_{it}((\tau^{-1}(g_k))^t + (\tau^{-1}(g_{k-1}))^t)\right) \\ &\quad +\frac{1}{2}B^{t,a}(x_k)\left(\ell^*_{g_{k-1}} D_3 L_d(x_{k-1}, x_k, g_{k-1}) + r^*_{g_k} D_3 L_d(x_k, x_{k+1}, g_k)\right)_t = 0,\end{aligned} \tag{36}$$

or, equivalently,

$$A^{i,a}(x_k)\left(\tilde{\mathfrak{G}}_{ij}\frac{(x^j_{k+1}-x^j_{k-1})}{2h}+\frac{1}{2}\tilde{\mathfrak{G}}_{it}(\xi^t_k+\xi^t_{k-1})\right)$$

$$\frac{1}{2}B^{t,a}(x_k)\left((\mathrm{d}\tau^{-1}_{-h\xi_{k-1}})^*D_3l_d(x_{k-1},x_k,h\xi_{k-1})+(\mathrm{d}\tau^{-1}_{h\xi_k})^*D_3l_d(x_k,x_{k+1},h\xi_k)\right)_t=0,$$

where

$$A^{i,a}(x_k)=(\tilde{\mathfrak{G}}^{-1})^{ij}\mu^a_j(x_k)+(\tilde{\mathfrak{G}}^{-1})^{it}\eta^a_t(x_k),$$
$$B^{t,a}(x_k)=(\tilde{\mathfrak{G}}^{-1})^{ti}\mu^a_i(x_k)+(\tilde{\mathfrak{G}}^{-1})^{ts}\eta^a_s(x_k),$$

$(\tilde{\mathfrak{G}}^{-1})$ being the inverse matrix of $(\tilde{\mathfrak{G}})=\begin{pmatrix}\tilde{\mathfrak{G}}_{ij} & \tilde{\mathfrak{G}}_{sj}\\ \tilde{\mathfrak{G}}_{it} & \tilde{\mathfrak{G}}_{st}\end{pmatrix}$.

Our aim in the following is to find an extension of the nonholonomic RATTLE algorithm presented in remark 5.1 for systems defined on $T\mathbb{R}^n\times\mathfrak{g}$. For that purpose we define $\tilde{p}_k, p_{k+1/2}\in T^*_{x_k}\mathbb{R}^n$ and $\tilde{M}_k, M_{k+1/2}\in\mathfrak{g}^*$ by

$$(\tilde{p}_k)_i=\tilde{\mathfrak{G}}_{ij}\frac{(x^j_{k+1}-x^j_{k-1})}{2h}+\frac{1}{2}\tilde{\mathfrak{G}}_{is}(\xi^s_k+\xi^s_{k-1}),$$
$$(p_{k+1/2})_i=\tilde{\mathfrak{G}}_{ij}\frac{(x^j_{k+1}-x^j_k)}{h}+\tilde{\mathfrak{G}}_{is}\xi^s_k,$$
$$\tilde{M}_k=(\mathrm{d}\tau^{-1}_{h\xi_k})^*D_3l_d(x_k,x_{k+1},h\xi_k),$$
$$M_{k+1/2}=\mathrm{Ad}^*_{\tau(h\xi_k)}\tilde{M}_k-\frac{1}{2}\lambda_{a,k+1}\,\eta^a_s(x_{k+1})\,E^s,$$

where $\tilde{\lambda}_{a,k}=\lambda_{a,k}/h$. We also recall that $\xi_k=\tau^{-1}(g_k)/h$. After these redefinitions, equations (33), (35) and (36) can be translated into the following algorithm

$$p_{k+1/2}=\tilde{p}_k-\frac{h}{2}\left(V_x(x_k)+\tilde{\lambda}_{a,k}\,\mu^a(x_k)\right),\qquad(37a)$$

$$M_{k+1/2}=\mathrm{Ad}^*_{\tau(h\xi_k)}\tilde{M}_k-\frac{1}{2}\lambda_{a,k+1}\,\eta^a(x_{k+1}),\qquad(37b)$$

$$x^i_{k+1}=x^i_k+h(\tilde{\mathfrak{G}}^{-1})^{ij}\left((p_{k+1/2})_j-\tilde{\mathfrak{G}}_{jt}\,\xi^t_k\right),\qquad(37c)$$

$$A^a(x_{k+1})\,\tilde{p}_{k+1}+\frac{1}{2}B^a(x_{k+1})\left(\mathrm{Ad}^*_{\tau(h\xi_k)}\,\tilde{M}_k+\tilde{M}_{k+1}\right)=0,\qquad(37d)$$

$$\tilde{p}_{k+1}=p_{k+1/2}-\frac{h}{2}\left(V_x(x_{k+1})+\tilde{\lambda}_{a,k+1}\,\mu^a(x_{k+1})\right),\qquad(37e)$$

$$\tilde{M}_{k+1}=M_{k+1/2}-\frac{1}{2}\lambda_{a,k+1}\,\eta^a(x_{k+1}),\qquad(37f)$$

with the natural definitions $\eta^a(x_k)=\eta^a_t(x_k)\,E^t$, $\mu^a(x_k)=\mu^a_i\,\mathrm{d}x^i$, $A^a(x_k)=A^{i,a}(x_k)\frac{\partial}{\partial x^i}$, $B^a(x_k)=B^{t,a}(x_k)E_t$; moreover, most of the equations are written in matrix form.

Next, we present the following sequence in order to obtain the 1-step values $(x_{k+1},\tilde{p}_{k+1},\xi_{k+1},\tilde{M}_{k+1},\tilde{\lambda}_{a,k+1})$ from the original values $(x_k,\tilde{p}_k,\xi_k,\tilde{M}_k,\tilde{\lambda}_{a,k})$. First, it is clear that $p_{k+1/2}$ is directly obtained from (37*a*). Once $p_{k+1/2}$ is fixed, the same happens in (37*c*) determining x_{k+1}. Moreover, introducing (37*b*) into (37*f*) we obtain the system of equations

$$0=A^a(x_{k+1})\,\tilde{p}_{k+1}+\frac{1}{2}B^a(x_{k+1})\left(\mathrm{Ad}^*_{\tau(h\xi_k)}\,\tilde{M}_k+\tilde{M}_{k+1}\right),$$
$$\tilde{p}_{k+1}=p_{k+1/2}-\frac{h}{2}\left(V_x(x_{k+1})+\tilde{\lambda}_{a,k+1}\,\mu^a(x_{k+1})\right),$$
$$\tilde{M}_{k+1}=\mathrm{Ad}^*_{\tau(h\xi_k)}\tilde{M}_k-\lambda_{a,k+1}\,\eta^a(x_{k+1}),$$

which implicitly provides $(\tilde{p}_{k+1}, \tilde{M}_{k+1}, \tilde{\lambda}_{a,k+1})$. Therefore, we see that equations (37) do not give the value ξ_{k+1} directly. Nevertheless, replacing (37*a*) into (37*c*) and taking a step forward, we obtain the equation

$$x_{k+2} = x_{k+1} + h(\tilde{\mathcal{G}}^{-1}) \left(\tilde{p}_{k+1} - \frac{h}{2} \left(V_x(x_{k+1}) + \tilde{\lambda}_{a,k+1}\, \mu^a(x_{k+1}) \right) - \tilde{\mathcal{G}}\, \xi_{k+1} \right),$$

which determines x_{k+2} in terms of $x_{k+1}, \tilde{p}_{k+1}, \tilde{\lambda}_{a,k+1}$ (already fixed by the previous sequence) and ξ_{k+1}. Finally, introducing this value of x_{k+2} into the definition of $\tilde{M}_{k+1}$ we obtain the equation

$$\tilde{M}_{k+1} = (\mathrm{d}\tau^{-1}_{h\xi_{k+1}})^* D_3 l_d(x_{k+1}, x_{k+2}, h\xi_{k+1}),$$

which implicitly determines ξ_{k+1} since $\tilde{M}_{k+1}$ has been previously determined. Note that this last step is not incompatible with equations (37) since the chosen value of x_{k+2}, and also $\tilde{M}_{k+1}$'s, is precisely the one that the algoritm provides. Schematically, the proposed algorithm can be represented by

$$(x_k, \tilde{p}_k, \xi_k, \tilde{M}_k, \tilde{\lambda}_{a,k}) \to (p_{k+1/2}, x_{k+1}) \to (\tilde{p}_{k+1}, \tilde{M}_{k+1}, \tilde{\lambda}_{a,k+1}) \to \xi_{k+1}.$$

Remark 7.2. A natural question related to the reduction of continuous or discrete mechanical systems with symmetry concerns the reverse procedure. Once the solutions of the reduced system have been obtained, how can we recover from them the solutions of the unreduced system? Observe that, in our case, we have only considered the case of trivial principal bundles $\mathrm{pr}_1 : M \times G \to M$ with trivial action $\Phi_{\tilde{W}}(x, W) = (x, \tilde{W}W)$ where $x \in M$ and $W, \tilde{W} \in G$. The original mechanical Lagrangian is defined by $L : T(M \times G) \equiv TM \times TG \to \mathbb{R}$ along with the nonholonomic distribution $\mathcal{D}$. The reduced system $(\tilde{L}, \tilde{\mathcal{D}})$ is defined on $TM \times \mathfrak{g}$ and, given a reduced solution of the nonholonomic system $(x(t), \xi(t))$, we can obtain the solution of the original system by solving additionally the equation $\dot{W}(t) = W(t)\xi(t)$, which is called the *reconstruction equation*. In the discrete case we have a similar scheme. Namely, a reduced solution is a sequence (x_k, x_{k+1}, g_k) and the discrete solutions $(x_k, x_{k+1}, W_k, W_{k+1})$ of the unreduced system are derived by the discrete reconstruction equation $W_{k+1} = W_k g_k$. Moreover, if we describe our reduced integrator using a retraction map $\tau : \mathfrak{g} \to G$, then the reconstruction equation reads $W_{k+1} = W_k \tau(h\xi_k)$.

7.3. The case of affine constraints

We consider in this section the extension of the reduced GNI method for the case of affine nonholonomic constraints. With the same notation as in section 7.1, take an affine bundle $\tilde{\mathcal{A}}$ of $TM \times \mathfrak{g}$ modelled on the vector bundle $\tilde{\mathcal{D}}$ and assume that there exists a globally defined section $\tilde{Y} \in \Gamma(TM \times \mathfrak{g})$ such that $v_x \in \tilde{\mathcal{A}}_x$ if and only if $v_x - \tilde{Y}(x) \in \tilde{\mathcal{D}}_x$.

Fixing a local basis of sections $\{e_I\} = \{\tilde{e}_\alpha, \tilde{e}_a\}$ of $\Gamma(TM \times \mathfrak{g})$ adapted to the orthogonal decomposition $\tilde{\mathcal{D}} \oplus \tilde{\mathcal{D}}^\perp$, the constraints determining locally the affine subbundle $\tilde{\mathcal{A}}$ are

$$y^a - Y^a(x) = 0,$$

where $\tilde{Y} = Y^\alpha \tilde{e}_\alpha + Y^a \tilde{e}_a$.

In our case, the initial data defining our *reduced nonholonomic affine problem* is denoted by the 4-tuple $(\tilde{\mathcal{D}}, \tilde{\mathcal{G}}, \tilde{Y}, \tilde{V})$ (see section 7.1). By means of the metric, from $\tilde{Y}$, we can uniquely define a 1-section $\tilde{\mathcal{G}}(\tilde{Y}, \cdot) = \Pi \in \Gamma(T^*M \times \mathfrak{g}^*)$. Locally, $\Pi = \tilde{\mathcal{G}}_{IJ} Y^J e^I$.

Consider a discrete Lagrangian $L_d : M \times M \times G \to \mathbb{R}$. As in the previous sections, we can split the total space E as $E = \tilde{\mathcal{D}} \oplus \tilde{\mathcal{D}}^\perp$ with corresponding projectors $\mathcal{P} : E \to \tilde{\mathcal{D}}$,

$\mathcal{Q} : E \to \tilde{\mathcal{D}}^\perp$. Thus, the proposed *reduced GNI equations* for affine constraints are a mixture of definitions 6.1 and 7.1, namely

$$\mathcal{P}^*_{x_k}\left(\mathbb{F}L_d^-(x_k, x_{k+1}, g_k)\right) - \mathcal{P}^*_{x_k}\left(\mathbb{F}L_d^+(x_{k-1}, x_k, g_{k-1})\right) = 0, \tag{38a}$$

$$\mathcal{Q}^*_{x_k}\left(\mathbb{F}L_d^-(x_k, x_{k+1}, g_k)\right) + \mathcal{Q}^*_{x_k}\left(\mathbb{F}L_d^+(x_{k-1}, x_k, g_{k-1})\right) + 2\mathcal{Q}^*_{x_k}\Pi = 0, \tag{38b}$$

where the Legendre transforms $\mathbb{F}L_d^\pm$ are defined in (29).

7.4. Example: the rolling ball

Consider the motion of an inhomogeneous sphere of radius $r > 0$ that rolls without slipping on a horizontal table. If the sphere is balanced, that is, the centre of mass of the sphere coincides with the geometric centre, we recover the well-known problem of the Chaplygin sphere. It is known that the Chaplygin sphere has an invariant measure and is therefore conformally Hamiltonian (see [9–11, 20] and references therein).

We consider here a balanced sphere and add the condition that the table is rotating with constant angular velocity Θ about a vertical axis.

The configuration space for the continuous system is $Q = \mathbb{R}^2 \times SO(3)$, with coordinates (x, y, R). The (x, y) coordinates are specified with respect to an inertial frame. The centre of rotation of the table is located at $(x, y) = (0, 0)$. The orthogonal matrix R gives the configuration of the sphere as a rotation with respect to a reference configuration where its principal axes of inertia are aligned with the coordinate axes. It is well known that there exists an isomorphism $\hat{\cdot} : \mathbb{R}^3 \to \mathfrak{so}(3)$ given by

$$\hat{z} = \begin{pmatrix} 0 & -z_3 & z_2 \\ z_3 & 0 & -z_1 \\ -z_2 & z_1 & 0 \end{pmatrix} \in \mathfrak{so}(3), \tag{39}$$

where $z = (z_1, z_2, z_3) \in \mathbb{R}^3$. Let $\hat{\omega} = \dot{R}R^{-1}$ and $\hat{\Omega} = R^{-1}\dot{R}$, so $\omega, \Omega \in \mathbb{R}^3$ represent the angular velocity in spatial and body coordinates respectively. It is easy to check that $\Omega = R^{-1}\omega$.

The Lagrangian function is determined by the total kinetic energy $L: T(\mathbb{R}^2 \times SO(3)) \to \mathbb{R}$, i.e.

$$L(x, y, R, \dot{x}, \dot{y}, \dot{R}) = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2) + \frac{1}{2}(I_1\,\Omega_1^2 + I_2\,\Omega_2^2 + I_3\,\Omega_3^2), \tag{40}$$

where Ω is computed from R and $\dot{R}$ as above. The nonholonomic constraints read

$$\dot{x} - r\,\omega_2 + \Theta\,y = 0, \tag{41a}$$

$$\dot{y} + r\,\omega_1 - \Theta\,x = 0. \tag{41b}$$

Clearly, these constraints are not linear but affine, except in the particular case where the table is fixed.

We will consider two cases. In the first one, the ball is homogeneous, that is, its three principal moments of inertia are equal. In the second case, we apply our method to the general situation of an inhomogeneous ball.

7.4.1. The homogeneous case. Assume that the three principal moments of inertia are equal, that is, $I = I_1 = I_2 = I_3$. If $\hat{\omega} = \dot{R}R^{-1}$ and $\hat{\Omega} = R^{-1}\dot{R}$ as before, then

$$L(x, y, R, \dot{x}, \dot{y}, \dot{R}) = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2) + \frac{1}{2}I\|\Omega\|^2 = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2) + \frac{1}{2}I\|\omega\|^2, \tag{42}$$

since $\Omega = R^{-1}\omega$ and $R \in SO(3)$. This induces a reduced Lagrangian $l : T\mathbb{R}^2 \times \mathfrak{so}(3) \to \mathbb{R}$ given by

$$l(x, y, \dot{x}, \dot{y}; \omega) = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2) + \frac{1}{2}I\|\omega\|^2.$$

Then we can apply the procedure developed in section 7.3 for reduced systems with affine nonholonomic constraints.

Define a global basis of sections of the reduced tangent bundle $E = T\mathbb{R}^2 \times \mathfrak{so}(3) \to \mathbb{R}^2$ by

$$\tilde{e}_1 = \left(\frac{\partial}{\partial x}, 0\right), \ \tilde{e}_2 = \left(\frac{\partial}{\partial y}, 0\right),$$
$$\tilde{e}_3 = (0, E_1), \ \tilde{e}_4 = (0, E_2), \ \tilde{e}_5 = (0, E_3),$$

where $\{E_1, E_2, E_3\}$ is the basis of $\mathfrak{so}(3)$ obtained from the standard basis of $\mathbb{R}^3$ via the isomorphism $\hat{\cdot}$. Denote its dual basis by $\{\tilde{e}^1, \ldots, \tilde{e}^5\}$. The distribution corresponding to the constraints (41) may be written as

$$\tilde{\mathcal{D}} = \operatorname{span}\{r\tilde{e}_1 + \tilde{e}_4, \ -r\tilde{e}_2 + \tilde{e}_3, \ \tilde{e}_5\},$$

while the section $\tilde{Y}$ of E is

$$\tilde{Y} = -\Theta\, y\, \tilde{e}_1 + \Theta\, x\, \tilde{e}_2.$$

The Lagrangian l determines the metric

$$\tilde{\mathcal{G}} = m(\tilde{e}^1 \otimes \tilde{e}^1 + \tilde{e}^2 \otimes \tilde{e}^2) + I(\tilde{e}^3 \otimes \tilde{e}^3 + \tilde{e}^4 \otimes \tilde{e}^4 + \tilde{e}^5 \otimes \tilde{e}^5).$$

With respect to this metric, the orthogonal complement to $\tilde{\mathcal{D}}$ is

$$\tilde{\mathcal{D}}^{\perp} = \operatorname{span}\left\{\tilde{e}_1 - \frac{mr}{I}\tilde{e}_4, \ \tilde{e}_2 + \frac{mr}{I}\tilde{e}_3\right\}.$$

The projection $\mathcal{Q} : T\mathbb{R}^2 \times \mathfrak{so}(3) \to \tilde{\mathcal{D}}^{\perp}$ is given in coordinates by the matrix

$$\mathcal{Q} = \begin{pmatrix} \frac{I}{mr^2+I} & 0 & 0 & \frac{-rI}{mr^2+I} & 0 \\ 0 & \frac{I}{mr^2+I} & \frac{rI}{mr^2+I} & 0 & 0 \\ 0 & \frac{mr}{mr^2+I} & \frac{mr^2}{mr^2+I} & 0 & 0 \\ \frac{-mr}{mr^2+I} & 0 & 0 & \frac{mr^2}{mr^2+I} & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \tag{43}$$

while $\mathcal{P} : T\mathbb{R}^2 \times \mathfrak{so}(3) \to \tilde{\mathcal{D}}$ is given by

$$\mathcal{P} = \begin{pmatrix} \frac{mr^2}{mr^2+I} & 0 & 0 & \frac{rI_2}{mr^2+I} & 0 \\ 0 & \frac{mr^2}{mr^2+I} & \frac{-rI_1}{mr^2+I} & 0 & 0 \\ 0 & \frac{-mr}{mr^2+I} & \frac{I_1}{mr^2+I} & 0 & 0 \\ \frac{mr}{mr^2+I} & 0 & 0 & \frac{I_2}{mr^2+I} & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \tag{44}$$

For a discrete Lagrangian $l_d : \mathbb{R}^2 \times \mathbb{R}^2 \times \mathfrak{so}(3) \to \mathbb{R}$, define the discrete reduced Legendre transformations $\mathbb{F}l_d^{\pm}$ as

$$\mathbb{F}l_d^{-} : \mathbb{R}^2 \times \mathbb{R}^2 \times \mathfrak{so}(3) \to T^*\mathbb{R}^2 \times \mathfrak{so}^*(3)$$
$$(q_k, q_{k+1}, \omega_k) \longmapsto (q_k, -D_1 l_d(q_k, q_{k+1}, \omega_k), (\mathrm{d}\tau^{-1}_{h\omega_k})^* D_3 l_d(q_k, q_{k+1}, \omega_k)),$$
$$\mathbb{F}l_d^{+} : \mathbb{R}^2 \times \mathbb{R}^2 \times \mathfrak{so}(3) \to T^*\mathbb{R}^2 \times \mathfrak{so}^*(3)$$
$$(q_k, q_{k+1}, \omega_k) \longmapsto (q_{k+1}, D_2 l_d(q_k, q_{k+1}, \omega_k), (\mathrm{d}\tau^{-1}_{-h\omega_k})^* D_3 l_d(q_k, q_{k+1}, \omega_k)).$$

The relationship between $\mathbb{F}L_d^{\pm}$ in equations (38) and $\mathbb{F}l_d^{\pm}$ is given by the properties of the retraction map τ presented in the Appendix (see [29] for more details). The proposed nonholonomic equations (38) become

$$\mathcal{P}^*_{q_k}\left(\mathbb{F}l_d^-(q_k, q_{k+1}, \omega_k)\right) - \mathcal{P}^*_{q_k}\left(\mathbb{F}l_d^+(q_{k-1}, q_k, \omega_{k-1})\right) = 0, \tag{45a}$$

$$\mathcal{Q}^*_{q_k}\left(\mathbb{F}l_d^-(q_k, q_{k+1}, \omega_k)\right) + \mathcal{Q}^*_{q_k}\left(\mathbb{F}l_d^+(q_{k-1}, q_k, \omega_{k-1})\right) + 2\mathcal{Q}^*_{q_k}\Pi = 0, \tag{45b}$$

where $q_k = (x_k, y_k) \in \mathbb{R}^2$, $\omega_k \in \mathfrak{so}(3)$ and $\Pi = \tilde{\mathcal{G}}(\tilde{Y}, \cdot)$, which in this case reads

$$\Pi = -m\Theta y\, \tilde{e}^1 + m\Theta x\, \tilde{e}^2.$$

We choose the discrete Lagrangian $l_d : \mathbb{R}^2 \times \mathbb{R}^2 \times \mathfrak{so}(3) \to \mathbb{R}$ as $l_d(q_k, q_{k+1}, \omega_k) = hl(q_k, \frac{q_{k+1}-q_k}{h}, \omega_k)$, that is,

$$l_d(q_k, q_{k+1}, \omega_k) = \frac{m}{2h}\left((x_{k+1} - x_k)^2 + (y_{k+1} - y_k)^2\right) + \frac{Ih}{2}\left((\omega_k)_1^2 + (\omega_k)_2^2 + (\omega_k)_3^2\right). \tag{46}$$

Setting the retraction map τ as the Cayley map for $SO(3)$, that is, $\tau(\omega) = \mathrm{cay}(\omega)$ (see the appendix for more details) and taking into account (46), (43) and (44), equations (45) read

$$mr\left(\frac{x_{k+1} - 2x_k + x_{k-1}}{h}\right) + I\left(\omega_2^k - \omega_2^{k-1}\right) + O_1(h^2) = 0,$$

$$mr\left(\frac{y_{k+1} - 2y_k + y_{k-1}}{h}\right) - I\left(\omega_1^k - \omega_1^{k-1}\right) + O_2(h^2) = 0,$$

$$I\left(\omega_3^k - \omega_3^{k-1}\right) + O_3(h^2) = 0,$$

$$\frac{x_{k+1} - x_{k-1}}{2h} + \Theta\, y_k - r\frac{\omega_2^k + \omega_2^{k-1}}{2} + O_4(h^2) = 0,$$

$$\frac{y_{k+1} - y_{k-1}}{2h} - \Theta\, x_k + r\frac{\omega_1^k + \omega_1^{k-1}}{2} + O_5(h^2) = 0,$$

where

$$O_1(h^2) = \frac{Ih^2}{4}\left(\omega_2^k\, ||\omega^k||^2 - \omega_2^{k-1}\, ||\omega^{k-1}||^2\right),$$

$$O_2(h^2) = -\frac{Ih^2}{4}\left(\omega_1^k\, ||\omega^k||^2 - \omega_1^{k-1}\, ||\omega^{k-1}||^2\right),$$

$$O_3(h^2) = \frac{Ih^2}{4}\left(\omega_3^k\, ||\omega^k||^2 - \omega_3^{k-1}\, ||\omega^{k-1}||^2\right),$$

$$O_4(h^2) = -\frac{h^2}{8}r\left(\omega_2^k\, ||\omega^k||^2 + \omega_2^{k-1}\, ||\omega^{k-1}||^2\right),$$

$$O_5(h^2) = \frac{h^2}{8}r\left(\omega_1^k\, ||\omega^k||^2 + \omega_1^{k-1}\, ||\omega^{k-1}||^2\right).$$

In these equations we recognize an order-one consistent discrete scheme for the continuous equations of the rolling ball system. This fact is not surprising since the discrete Lagrangian (46) is an order-one approximation of the action integral defined by the continuous Lagrangian (40) as well (see [43, 48] for more details regarding the relationship between the order of consistency of the discrete Lagrangian with respect to the action integral and of the variational integrators obtained from them).

In figure 1 we show the numerical results of applying this discrete method. We consider a homogeneous ball with $I = 2/3$, and $m = r = \Omega = 1$. We take decreasing values of the time step h, and compare to the method in [28]. We show errors with respect to the exact solution to the continuous system, with initial conditions $(x_0, y_0, \dot{x}_0, \dot{y}_0) = (1, 1, 1, 1)$, $\omega = (0, 2, 0)$, and a total run time of 10. Figure 2 shows the evolution of the x_k, y_k variables for these same physical parameters and initial conditions, for a total run time of 1000.

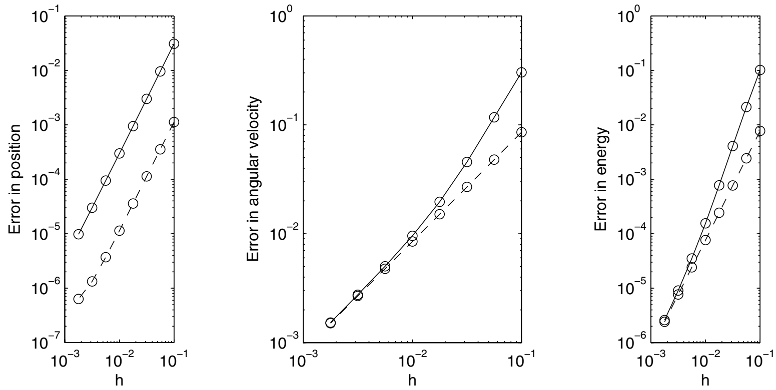

Figure 1. Errors in position (x, y), angular velocity ω and energy. The continuous line corresponds to the proposed method. The dashed line corresponds to the method in [28].

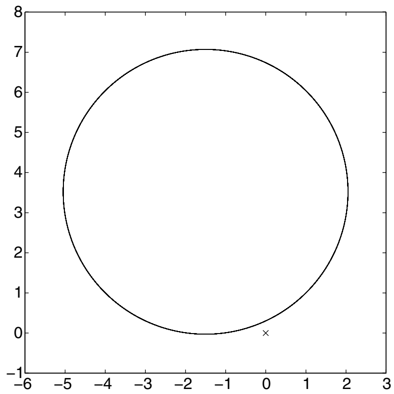

Figure 2. Position (x, y) for the point of contact of the homogeneous ball, with $h = 0.1$ and 10 000 steps. The cross indicates the centre of the rotating plate.

7.4.2. The inhomogeneous case. In the general case, we cannot write the Lagrangian as (42), so we need to work with the Lagrangian (40) expressed in terms of the body angular velocity, while the constraints (41) are expressed in terms of the spatial angular velocity. We have run simulations of the (not reduced) affine system on $Q = \mathbb{R}^2 \times SO(3)$ by pulling it back to $\mathbb{R}^2 \times \mathbb{R}^3$ using the map $\Xi\colon (x, y, \rho) \mapsto (x, y, \exp(\hat{\rho}))$, where $\exp\colon \mathfrak{so}(3) \to SO(3)$ is the exponential map. It is possible to show that

$$\Omega = \frac{\cos\|\rho\|-1}{\|\rho\|^2}\rho \times \dot{\rho} - \frac{\sin\|\rho\|-\|\rho\|}{\|\rho\|^3}(\rho \cdot \dot{\rho})\rho + \frac{\sin\|\rho\|}{\|\rho\|}\dot{\rho},$$
$$\omega = \frac{\cos\|\rho\|-1}{\|\rho\|^2}\dot{\rho} \times \rho - \frac{\sin\|\rho\|-\|\rho\|}{\|\rho\|^3}(\rho \cdot \dot{\rho})\rho + \frac{\sin\|\rho\|}{\|\rho\|}\dot{\rho}.$$

Using these expressions, we obtain the pullbacks of the Lagrangian and of the constraints in terms of $(x, y, \rho, \dot{x}, \dot{y}, \dot{\rho})$.

The nonholonomic integrator is then applied to this system. We have taken the very simple discrete Lagrangian

$$L_d(x_k, y_k, \rho_k, x_{k+1}, y_{k+1}, \rho_{k+1}) = h(\Xi^* L)\left(x_k, y_k, \rho_k, \frac{x_{k+1}-x_k}{h}, \frac{y_{k+1}-y_k}{h}, \frac{\rho_{k+1}-\rho_k}{h}\right),$$

where, for each k, $(x_k, y_k) \in \mathbb{R}^2$ and $\rho_k \in \mathbb{R}^3$. The metric and projections are not constant, unlike in the previous case. The discrete equations are derived using (26). Even though their

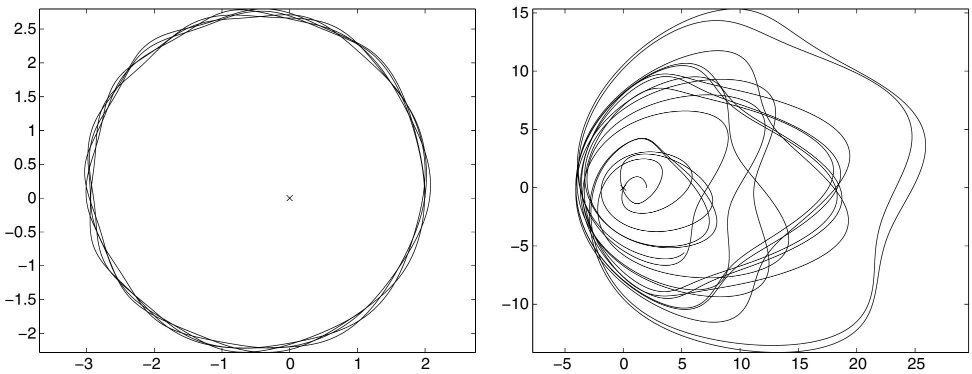

Figure 3. Position of the point of contact for an inhomogeneous sphere on a rotating table. Left: $I_1 = 1$, $I_2 = .5$, $I_3 = .7$, $m = 2$. Right: $I_1 = 10$, $I_2 = 10$, $I_3 = 1$, $m = 1$ (not physically valid). The centre of rotation of the table is indicated with a cross at $(0, 0)$. The two larger loops are not consecutive in time.

computation is straightforward using a computer algebra system, the resulting expressions are too long to include here.

In figure 3 we show simulations of the trajectory of the point of contact using this method. For the left plot we have used $I_1 = 1$, $I_2 = 0.5$, $I_3 = 0.7$, $m = 2$, $r = 1$ and $\Theta = 1$. The time step is $h = 2.5 \times 10^{-4}$, with a total run time of 100. The initial conditions for the discrete algorithm are $x_0 = 1$, $y_0 = 0$, $x_1 = x_0$, $y_1 = y_0 + 0.75h$, $\rho_0 = (0.5, 0.5, 0.5)$, and ρ_1 computed using an appropriate discretization of the nonholonomic constraints. A video of this simulation, up to time 40, can be found at vimeo.com/114869680. On the right of the same figure, we used $I_1 = 10$, $I_2 = 10$, $I_3 = 1$, $m = 1$ and $h \approx 1.7783 \times 10^{-4}$, with a total run time of 160. These values do not correspond to a physically valid mass distribution since they would require some mass to be located *outside* the surface of the sphere; nevertheless, we include this simulation as it shows an interesting qualitative behaviour of the solution. A video up to time 40 can be found at vimeo.com/114869682.

Figure 4 shows the error in energy for the case of an inhomogeneous sphere and a fixed table. We compare the energy of the discrete trajectory with the constant energy of the exact solution.

8. Extension to Lie algebroids

8.1. Brief introduction to Lie groupoids and Lie algebroids

Definition 8.1. A *Lie groupoid*, denoted $G \rightrightarrows Q$, consists of two differentiable manifolds G and Q and the following differentiable maps (the structural maps):

(1) A pair of submersions: the *source map* $\alpha\colon G \to Q$ and the *target map* $\beta\colon G \to Q$.
(2) An associative *multiplication map* $m\colon G_2 \to G$, $(g, h) \mapsto gh$, where the set

$$G_2 = \{(g, h) \in G \times G \;\;||\;\; \beta(g) = \alpha(h)\}$$

is called the set of *composable pairs*.
(3) An *identity section* $\epsilon\colon Q \to G$ of α and β, such that for all $g \in G$,

$$\epsilon\left(\alpha(g)\right) g = g = g\epsilon\left(\beta(g)\right).$$

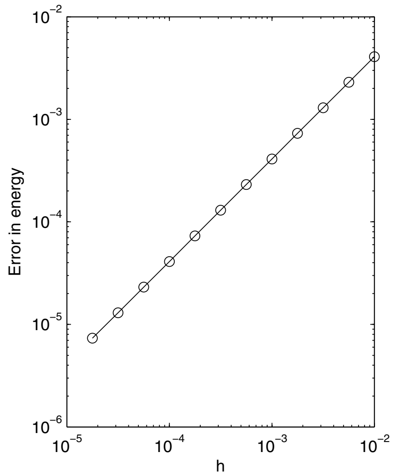

Figure 4. Error in energy for $I_1 = 1$, $I_2 = 0.5$, $I_3 = 0.7$ (inhomogeneous sphere), $m = 2$, $r = 1$, $\Theta = 0$ (fixed table), for a total run time of 10 and initial conditions such that the sphere rolls a distance of about 16 units.

(4) An *inversion map* $i\colon G \to G$, $g \mapsto g^{-1}$, such that for all $g \in G$,

$$gg^{-1} = \epsilon(\alpha(g)), \qquad g^{-1}g = \epsilon(\beta(g)).$$

Next, we will introduce the notion of a left (right) translation by an element of a Lie groupoid. Given a groupoid $G \rightrightarrows Q$ and an element $g \in G$, define the **left translation** $\ell_g\colon \alpha^{-1}(\beta(g)) \to \alpha^{-1}(\alpha(g))$ and **right translation** $r_g\colon \beta^{-1}(\alpha(g)) \to \beta^{-1}(\beta(g))$ by g to be

$$\ell_g(h) = gh, \qquad r_g(h) = hg.$$

Analogously to the case of Lie groups, one may introduce the notion of left (right)-invariant vector field in a Lie groupoid from these translations. Given a Lie groupoid $G \rightrightarrows Q$, a vector field $\xi \in \mathfrak{X}(G)$ is *left-invariant* if ξ is α-vertical and $(T_h\ell_g)(\xi(h)) = \xi(gh)$ for all $(g, h) \in G_2$. Similarly, ξ is *right-invariant* if ξ is β-vertical and $(T_h r_g)(\xi(h)) = \xi(hg)$ for all $(h, g) \in G_2$.

It is well known that there always exists a Lie algebroid associated to a Lie groupoid (again analogously to the Lie group case). We consider the vector bundle $\tau_{AG} : AG \to Q$, whose fibre at a point $x \in Q$ is $(AG)_x = V_{\epsilon(x)}\alpha = \ker(T_{\epsilon(x)}\alpha)$. It is easy to prove that there exists a bijection between the space $\Gamma(\tau)$ and the set of left (right)-invariant vector fields on G. If X is a section of $\tau_{AG} : AG \to Q$, the corresponding left (right)-invariant vector field on G will be denoted $\overleftarrow{X}$ (respectively, $\overrightarrow{X}$), where

$$\overleftarrow{X}(g) = (T_{\epsilon(\beta(g))}\ell_g)(X(\beta(g))),$$
$$\overrightarrow{X}(g) = -(T_{\epsilon(\alpha(g))}r_g)((T_{\epsilon(\alpha(g))}i)(X(\alpha(g)))),$$

for $g \in G$. Using the above facts, we may introduce a *Lie algebroid structure* $([\![\cdot,\cdot]\!], \rho)$ on AG, which is defined by

$$\overleftarrow{[\![X, Y]\!]} = [\overleftarrow{X}, \overleftarrow{Y}], \quad \rho(X)(x) = (T_{\epsilon(x)}\beta)(X(x)),$$

for $X, Y \in \Gamma(\tau)$ and $x \in Q$. Note that

$$\overrightarrow{[\![X, Y]\!]} = -[\overrightarrow{X}, \overrightarrow{Y}], \quad [\overrightarrow{X}, \overleftarrow{Y}] = 0$$

(for more details, see [40]).

8.2. GNI extension to Lie groupoids

Let $G \rightrightarrows Q$ be a Lie groupoid and $\tau_{AG} : AG \to Q$ its associated Lie algebroid.

Consider a mechanical system subjected to linear nonholonomic constraints, that is, a pair $(L, \mathcal{D})$ (see [44, 28] for more details), where

(i) $L : AG \to \mathbb{R}$ is a Lagrangian function of mechanical type

$$L(a) = \frac{1}{2}\,\mathcal{G}(a, a) - V(\tau_{AG}(a)), \quad \text{where } a \in AG.$$

(ii) $\mathcal{D}$ is the total space of a vector subbundle $\tau_{\mathcal{D}} : \mathcal{D} \to Q$ of AG.

Here $\mathcal{G} : AG \times_Q AG \to \mathbb{R}$ is a bundle metric on AG. We also consider the orthogonal decomposition $AG = \mathcal{D} \oplus \mathcal{D}^\perp$ and the associated projectors

$$\mathcal{P} : AG \to \mathcal{D} \qquad \text{and} \qquad \mathcal{Q} : AG \to \mathcal{D}^\perp. \tag{47}$$

Consider a discretization $L_d : G \to \mathbb{R}$ of the Lagrangian L. It is possible to define two Legendre transformations $\mathbb{F}L_d^\pm : G \to A^*G$ by

$$\begin{aligned} \mathbb{F}L_d^-(h)(v_{\epsilon(\alpha(h))}) &= -v_{\epsilon(\alpha(h))}(L_d \circ r_h \circ i), \\ \mathbb{F}L_d^+(g)(v_{\epsilon(\beta(g))}) &= v_{\epsilon(\beta(g))}(L_d \circ \ell_g), \end{aligned} \tag{48}$$

where $v_{\epsilon(\alpha(h))} \in A_{\alpha(h)}G$ and $v_{\epsilon(\beta(g))} \in A_{\beta(g)}G$. Therefore $\mathbb{F}L_d^-(h) \in A^*_{\alpha(h)}G$ and $\mathbb{F}L_d^+(g) \in A^*_{\beta(g)}G$. Since the Euler–Lagrange equations are given by the matching of momenta, in the Lie groupoid setting they read

$$\mathbb{F}L_d^-(h) = \mathbb{F}L_d^+(g),$$

where (g, h) is in the set G_2.

Definition 8.2. Consider the projectors (47) and the discrete Legendre transforms $\mathbb{F}L_d^\pm$ (48). The extension of the GNI method for Lie algebroids is defined by the equations

$$\mathcal{P}_q^*\left(\mathbb{F}L_d^-(h) - \mathbb{F}L_d^+(g)\right) = 0 \tag{49a}$$

$$\mathcal{Q}_q^*\left(\mathbb{F}L_d^-(h) + \mathbb{F}L_d^+(g)\right) = 0, \tag{49b}$$

where the subscript q emphasizes the fact that the projections take place in the fibre over $q = \alpha(h) = \beta(g)$.

Let $\{X_\alpha, X_a\}$ be a local basis adapted to $\mathcal{D} \oplus \mathcal{D}^\perp$, in the sense that locally $\mathcal{D} = \text{span}\{X_\alpha\}$ and $\mathcal{D}^\perp = \text{span}\{X_a\}$. We can rewrite equations (49) as

$$\mathbb{F}L_d^-(h)\,(X_\alpha(q)) - \mathbb{F}L_d^+(g)\,(X_\alpha(q)) = 0, \tag{50a}$$

$$\mathbb{F}L_d^-(h)\,(X_a(q)) + \mathbb{F}L_d^+(g)\,(X_a(q)) = 0, \tag{50b}$$

where $\alpha(h) = \beta(g) = q \in Q$ (so $(g, h) \in G_2$). Let us denote

$$p_g^+ = \mathbb{F}L_d^+(g) \in A_q^*G,$$

$$p_h^- = \mathbb{F}L_d^-(h) \in A_q^*G,$$

so equation (50*b*) becomes

$$\left(\frac{p_g^+ + p_h^-}{2}\right)(X_a(q)) = 0.$$

If $\mu^a \in \Gamma(A^*G)$ are such that $\mathcal{D}^\circ = \text{span}\{\mu^a\}$, then this last equation becomes

$$\mathcal{G}\left(\frac{p_g^+ + p_h^-}{2}, \mu^a\right) = 0,$$

where, by a slight abuse of notation, we denote the bundle metric on A^*G naturally induced by the bundle metric on AG using the same symbol $\mathcal{G}$. Note that the set of $\eta \in A^*G$ such that $\mathcal{G}(\eta, \mu^a) = 0$ for all a forms the constraint submanifold $\mathcal{D} = \text{Leg}_{\mathcal{G}}(\mathcal{D})$. Therefore the average momentum $\tilde{p} = (p_g^+ + p_h^-)/2 \in \mathcal{D}$ satisfies in this sense the constraint equations.

9. Conclusions

In this paper, we continue the study of the properties of the geometric nonholonomic integrator (GNI) and extending the construction given in our previous work [23] to a more extense class of nonholonomic systems (reduced systems and systems with affine constraints). Our paper shows the importance of combining different research areas (differential geometry, numerical analysis and mechanics) to produce new geometric integrators for nonholonomic dynamics.

Such issues raise a number of future work directions. We therefore close with some open questions and future work:

- In future work, we will perform simulations applying our techniques to new families of nonholonomic systems. Specifically, we want to test our geometric integrator on different nonintegrable nonholonomic systems.
- Given a geometric nonholonomic integrator, does there exist, in the sense of backward error analysis, a continuous nonholonomic system, such that the discrete evolution for the nonholonomic integrator is the flow of this nonholonomic system up to an appropriate order?
- Is it possible to use the GNI in order to design numerical methods for optimal control of nonholonomic systems using the techniques developed in [29]? Furthermore, with these methods is even possible to approximate piecewise-smooth control, giving a more realistic behaviour. See also [3, 8, 53].
- Construction of new methods that mimic the so-called 'sister' piecewise holonomic system and study its relationship with the GNI method. The study of 'sister' systems is interesting to modellize the dynamics of human walking, and in an averaged sense they approach to nonholonomic systems (see for more information [26, 51, 52, 49] and references therein). Observe that GNI is related to an elastic impact with the nonholonomic distribution (see [23]).

Acknowledgments

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Appendix. Retraction maps

As mentioned in section 7.2 a *retraction map* $\tau : \mathfrak{g} \to G$ is an analytic local diffeomorphism which maps a neighbourhood of $0 \in \mathfrak{g}$ onto a neighbourhood of the neutral element $e \in G$, such that $\tau(0) = e$ and $\tau(\xi)\tau(-\xi) = e$, for $\xi \in \mathfrak{g}$. There are many choices for the map τ such as the Cayley map, the exponential map, etc. The retraction map is used to express small discrete changes in the group configuration through unique Lie algebra elements, say $\xi_k = \tau^{-1}(g_k^{-1} g_{k+1})/h$. That is, if ξ_k were regarded as an average velocity between g_k and g_{k+1}, then τ is an approximation to the integral flow of the dynamics. The difference $g_k^{-1} g_{k+1} \in G$, which is an element of a nonlinear space, can now be represented by the vector ξ_k. (See [12, 30] for further details.)

Of great importance is the *right trivialized tangent* of the retraction map. The following definition is complementary to (34).

Definition 9.1. Given a retraction map $\tau: \mathfrak{g} \to G$, its right trivialized tangent $\mathrm{d}\tau_\xi: \mathfrak{g} \to \mathfrak{g}$ is defined as the ξ-dependent linear map obtained by composition of the linear maps

$$\underbrace{\mathfrak{g} \xrightarrow{\{\xi\}\times \mathrm{id}} \{\xi\} \times \mathfrak{g} \xrightarrow{T_\xi \tau} T_{\tau(\xi)}G \xrightarrow{T_{\tau(\xi)} r_{\tau(\xi)^{-1}}} T_e G}_{\mathrm{d}\tau_\xi} \equiv \mathfrak{g}$$

where r denotes right translation in the group. Since τ is a local diffeomorphism, all the arrows are linear isomorphisms. We denote the inverse of $\mathrm{d}\tau_\xi$ as $\mathrm{d}\tau_\xi^{-1}$. Omitting the first identification for brevity, we can write

$$\mathrm{d}\tau_\xi \quad = T_{\tau(\xi)} r_{\tau(\xi)^{-1}} \circ T_\xi \tau \tag{51}$$

$$\mathrm{d}\tau_\xi^{-1} = (T_\xi \tau)^{-1} \circ T_e r_{\tau(\xi)} = T_{\tau(\xi)}(\tau^{-1}) \circ T_e r_{\tau(\xi)} \tag{52}$$

Remark 9.2. Omitting the identifications $\mathfrak{g} \equiv \{\xi\} \times \mathfrak{g}$, $\xi \in \mathfrak{g}$, can lead to mismatches when using the definitions above explicitly; for example, if we rewrite equation (54) below using (52), then the left-hand side would be in $\{\xi\} \times \mathfrak{g}$ while the right-hand side would be in $\{-\xi\} \times \mathfrak{g}$. This should cause no problems if the identifications are made explicit when needed. In any case, (54) makes sense as an identity in $\mathfrak{g}$.

Lemma 9.3. *(See [42]). Let $g \in G$, $\lambda \in \mathfrak{g}$ and δf denote the variation of a function f with respect to its parameters. Assuming λ is constant, the following identity holds:*

$$\delta(\mathrm{Ad}_g \lambda) = -\mathrm{Ad}_g [\lambda\,,\ g^{-1}\delta g],$$

where $[\cdot\,,\ \cdot] : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ denotes the Lie bracket operation or equivalently $[\xi\,,\ \eta] \equiv \mathrm{ad}_\xi \eta$, for given η, $\xi \in \mathfrak{g}$.

Lemma 9.4. *For each $\lambda \in \mathfrak{g}$, the derivative of the map $\psi_\lambda: \mathfrak{g} \to \mathfrak{g}$ defined by $\psi_\lambda(\xi) = \mathrm{Ad}_{\tau(\xi)}\lambda$ is given by*

$$D\psi_\lambda(\xi) \cdot \eta = -[\mathrm{Ad}_{\tau(\xi)}\lambda\,,\ \mathrm{d}\tau_\xi(\eta)],$$

$\eta \in \mathfrak{g}$.

Proof. By lemma 9.3,

$$\begin{aligned} D\psi_\lambda(\xi) \cdot \eta &= -\mathrm{Ad}_{\tau(\xi)}[\lambda\,,\ \tau(\xi)^{-1} T_\xi \tau(\eta)] \\ &= -[\mathrm{Ad}_{\tau(\xi)}\lambda\,,\ T_\xi \tau(\eta)\tau(\xi)^{-1}] \\ &= -[\mathrm{Ad}_{\tau(\xi)}\lambda\,,\ \mathrm{d}\tau_\xi(\eta)], \end{aligned}$$

obtained from the trivialized tangent definition 9.1 and using the fact that $\mathrm{Ad}_g[\lambda\,,\ \eta] = [\mathrm{Ad}_g\lambda\,,\ \mathrm{Ad}_g\eta]$. □

The lemma above holds not only for retraction maps but also for any smooth map $\tau: \mathfrak{g} \to G$, for which $\mathrm{d}\tau_\xi$ can be defined as in definition 9.1.

The following lemma relates the right trivialized tangents at ξ and $-\xi$, as well as their inverses.

Lemma 9.5. *For a retraction map $\tau: \mathfrak{g} \to G$ and any $\xi, \eta \in \mathfrak{g}$, the following identities hold:*

$$\mathrm{d}\tau_\xi\, \eta \quad = \mathrm{Ad}_{\tau(\xi)}\, \mathrm{d}\tau_{-\xi}\, \eta, \tag{53}$$

$$\mathrm{d}\tau_\xi^{-1}\, \eta = \mathrm{d}\tau_{-\xi}^{-1} \left(\mathrm{Ad}_{\tau(-\xi)}\, \eta\right). \tag{54}$$

Proof. Define $\rho(\xi) = \tau(\xi)^{-1}$. Differentiating and using definition 9.1, we get

$$T\rho(\xi)\cdot\eta = -T\ell_{\tau(\xi)^{-1}}\left(Tr_{\tau(\xi)^{-1}}\left(T\tau(\xi)\cdot\eta\right)\right) = -T\ell_{\tau(\xi)^{-1}}\left(\mathrm{d}\tau_\xi(\eta)\right),$$

where $T\ell$, Tr are the tangent of the left and right translations in the group respectively. On the other hand, we also have $\rho(\xi) = \tau(-\xi)$, so the chain rule implies

$$T\rho(\xi)\cdot\eta = T\tau(-\xi)\cdot(-\eta) = Tr_{\tau(-\xi)}(\mathrm{d}\tau_{-\xi}(-\eta)) = -Tr_{\tau(\xi)^{-1}}(\mathrm{d}\tau_{-\xi}(\eta)).$$

Equating both expressions we obtain (53).

For the second identity, replace η by $\mathrm{d}\tau_\xi^{-1}\,\eta$ in (53) to obtain

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

Solving for $\mathrm{d}\tau_\xi^{-1}\,\eta$, we obtain (54). □

Some retraction map choices

(a) The exponential map $\exp : \mathfrak{g} \to G$, defined by $\exp(\xi) = \gamma(1)$, where $\gamma : \mathbb{R} \to G$ is the integral curve through the identity of the vector field associated with $\xi \in \mathfrak{g}$ (hence, with $\dot\gamma(0) = \xi$). The right trivialized derivative and its inverse are

$$\mathrm{dexp}_x\, y = \sum_{j=0}^{\infty} \frac{1}{(j+1)!}\,\mathrm{ad}_x^j\, y,$$

$$\mathrm{dexp}_x^{-1}\, y = \sum_{j=0}^{\infty} \frac{B_j}{j!}\,\mathrm{ad}_x^j\, y,$$

where B_j are the Bernoulli numbers (see [25]). Typically, these expressions are truncated in order to achieve a desired order of accuracy.

(b) The Cayley map $\mathrm{cay} : \mathfrak{g} \to G$ is defined by $\mathrm{cay}(\xi) = (e - \frac{\xi}{2})^{-1}(e + \frac{\xi}{2})$ and is valid for a general class of *quadratic groups*. The quadratic Lie groups are those defined as

$$G = \left\{ Y \in GL(n, \mathbb{R}) \mid Y^T P Y = P \right\},$$

where $P \in GL(n, \mathbb{R})$ is a given matrix (here, $GL(n, \mathbb{R})$ denotes the general linear group of degree n). $O(n)$ or $SO(n)$ are examples of quadratic Lie groups. The corresponding Lie algebra is

$$\mathfrak{g} = \left\{ \Omega \in \mathfrak{gl}(n, \mathbb{R}) \mid P\Omega + \Omega^T P = 0 \right\}.$$

The right trivialized derivative and inverse of the Cayley map are defined by

$$\mathrm{dcay}_x\, y = \left(e - \frac{x}{2}\right)^{-1} y \left(e + \frac{x}{2}\right)^{-1},$$

$$\mathrm{dcay}_x^{-1}\, y = \left(e - \frac{x}{2}\right) y \left(e + \frac{x}{2}\right).$$

Applications to matrix groups: SO(3)

We specify the exact form of the Cayley transform for the group $SO(3)$. While we have given more than one general choice for τ, for computational efficiency we recommend the Cayley map since it is simple. In addition, it is suitable for iterative integration and optimization problems since its derivatives do not have any singularities that might otherwise cause difficulties for gradient-based methods. The group of rigid body rotations is represented by 3×3 matrices with orthonormal column vectors corresponding to the axes of a right-handed frame attached to the body. Recall the map $\hat{\cdot} : \mathbb{R}^3 \to \mathfrak{so}(3)$ presented in (39). A Lie algebra basis for $SO(3)$ can be constructed as $\{\hat{e}_1, \hat{e}_2, \hat{e}_3\}$, $\hat{e}_i \in \mathfrak{so}(3)$, where $\{e_1, e_2, e_3\}$ is the standard basis for $\mathbb{R}^3$. Elements $\xi \in \mathfrak{so}(3)$ can be identified with the vector $\omega \in \mathbb{R}^3$ through $\xi = \omega^\alpha \hat{e}_\alpha$, or $\xi = \hat{\omega}$. Under such identification the Lie bracket coincides with the standard cross product, i.e. $\mathrm{ad}_{\hat{\omega}} \hat{\rho} = \omega \times \rho$, for $\omega, \rho \in \mathbb{R}^3$. Using this identification we have

$$\mathrm{cay}(\hat{\omega}) = I_3 + \frac{4}{4+ \parallel \omega \parallel^2} \left(\hat{\omega} + \frac{\hat{\omega}^2}{2} \right),$$

where I_3 is the 3×3 identity matrix. The linear maps $\mathrm{d}\tau_\xi$ and $\mathrm{d}\tau_\xi^{-1}$ are expressed as the 3×3 matrices

$$\mathrm{dcay}_\omega = \frac{2}{4+ \parallel \omega \parallel^2}(2I_3 + \hat{\omega}), \quad \mathrm{dcay}_\omega^{-1} = I_3 - \frac{\hat{\omega}}{2} + \frac{\omega\,\omega^T}{4}.$$

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