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DISCRETE SECOND ORDER CONSTRAINED LAGRANGIAN SYSTEMS: FIRST RESULTS

NICOLÁS BORDA^{1,2,3}, JAVIER FERNÁNDEZ¹ AND SERGIO GRILLO^{1,3}

¹Instituto Balseiro, Universidad Nacional de Cuyo – C.N.E.A.
Av. Bustillo 9500, San Carlos de Bariloche, R8402AGP, República Argentina

²Departamento de Matemática, Facultad de Ciencias Exactas, Universidad Nacional de La Plata 50 y 115, La Plata, Buenos Aires, 1900, República Argentina

³Consejo Nacional de Investigaciones Científicas y Técnicas, República Argentina

ABSTRACT. We briefly review the notion of second order constrained (continuous) system (SOCS) and then propose a discrete time counterpart of it, which we naturally call discrete second order constrained system (DSOCS). To illustrate and test numerically our model, we construct certain integrators that simulate the evolution of two mechanical systems: a particle moving in the plane with prescribed signed curvature, and the inertia wheel pendulum with a Lyapunov constraint. In addition, we prove a local existence and uniqueness result for trajectories of DSOCSs. As a first comparison of the underlying geometric structures, we study the symplectic behavior of both SOCSs and DSOCSs.

1. Introduction

Discrete Variational Mechanics originated in the 60's, motivated by the construction of variational numerical integrators for the equations of motion of (continuous) mechanical systems. Since then, significant progress has been made in the study of discrete time versions of unconstrained systems and systems with holonomic constraints. The advantage offered by the resulting integrators, compared to other numerical methods, is that they take into account the underlying geometric structure present in the mechanical problem and, therefore, can be designed to respect, in some way, the momentum, energy, or symplectic structure (see [26] and the multiple references therein). The discrete dynamics in the more general case of nonholonomic constraints¹ was introduced more recently, in 2001, by J. Cortés and S. Martínez in [11]. Nonholonomic integrators have become of interest mainly because of their good performance in numerical experiments (see, for instance, [27, 5]). Still, they are less understood theoretically than the preceding ones.

Even broader than the continuous nonholonomic case, we have mechanical systems with higher order constraints, which have been studied in [7, 8, 21]. They are

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¹Classical references for (continuous) nonholonomic systems are [16, 28]. More recent ones are [3, 12].

Lagrangian systems with constraints involving higher order derivatives of the position. They have been considered for describing some simplified models of rolling viscoelastic bodies and systems with friction [8, 7]. They have also appeared in applications to the control of underactuated mechanical systems [21, 18, 20] (see Section 4.2). Such applications consist in finding constraints that ensure the desired behavior of the system under consideration and, then, taking the related constraint force as the control law (see also [25, 6, 30]). It is a general fact that every control signal can be obtained by this procedure using second order constraints [18]. For example, for asymptotic stabilization of underactuated systems Lyapunov constraints can be used (see [20] and Section 4.2).

It is worth remarking that the constraints appearing in most of the interesting applications, like those previously mentioned, involve, at most, second order derivatives, *i.e.* positions, velocities and accelerations. For this reason, we will only consider systems with (at most) second order constraints in this work.

The practical difficulty of solving the equations of motion of (continuous) mechanical systems with nonholonomic constraints leads to the numerical integrators mentioned above. The aim of this paper is to propose a discrete time counterpart of the (continuous) second order constrained Lagrangian systems. We study some basic properties of those discrete time systems and use them to construct numerical integrators for the continuous ones.

The plan for the paper is as follows. In Section 2 we review the notion of (continuous) second order constrained Lagrangian system. In addition, we prove a result characterizing the evolution with the flow of the natural Lagrangian symplectic structure of such a system. In Section 3 we introduce the discrete second order constrained Lagrangian systems, their dynamics and their equations of motion. In Sections 4.1 and 4.2 we apply the discrete formalism just developed to two examples. There we find numerical integrators and test their quality by comparing against either the exact solution or a well known integrator of the corresponding continuous system. On the other hand, in Section 5 we prove some results about the dynamics of the discrete systems: the existence of a well defined local flow and a discrete analogue of the evolution of the symplectic form studied in Section 2. Last, in Section 6, we comment on some directions of future work.

Notation: throughout the paper τ_X is the projection of the tangent bundle TX onto X.

2. Second order constrained Lagrangian systems

In this section we review the notion of higher order constrained system such as it appears in [7, 19]. In particular, we shall only consider first order Lagrangian functions (this partially excludes the systems studied in [23]). The focus of our exposition is on systems with constraints of order at most 2 for the reason explained in Section 1. Recall that $T^{(2)}Q$ denotes the second order tangent bundle of the manifold Q (see [13, 15]).

Definition 2.1 (SOCS). A second order constrained Lagrangian system is a quadruple (Q, L, C_K, C_V) where

- (1) Q is a finite dimensional differentiable manifold, the *configuration space*,
- (2) $L: TQ \to \mathbb{R}$ is a smooth function on the tangent bundle of Q, the Lagrangian,

- (3) $C_K \subset T^{(2)}Q$ is a submanifold, the kinematic constraints, and
- (4) $C_V \subset T^{(2)}Q \times_Q TQ$ (where \times_Q denotes the fiber product on Q) is such that for every $q \in Q$ and $\eta \in T_q^{(2)}Q$, the set $C_V|_{\eta} := C_V \cap (\{\eta\} \times T_q Q)$, naturally identified with a subset of $T_q Q$, is either empty or a vector subspace, the virtual displacements or variational constraints.

For every system of this type, the action functional is defined by $S(\gamma) := \int_{t_0}^{t_1} L(\gamma'(t)) dt$, where $\gamma : [t_0, t_1] \to Q$ is a smooth curve in Q and $\gamma'(t) \in TQ$ is its velocity (in what follows, $\gamma^{(2)} : [t_0, t_1] \to T^{(2)}Q$ will denote its 2-lift). An infinitesimal variation of γ is a smooth curve $\delta \gamma : [t_0, t_1] \to TQ$ such that $\tau_Q(\delta \gamma(t)) = \gamma(t) \forall t$, and it is said to have vanishing end points if $\delta \gamma(t_0) = 0$ and $\delta \gamma(t_1) = 0$. The dynamics of a SOCS is determined by the following Principle.

Definition 2.2 (Lagrange–d'Alembert's Principle for SOCSs). A smooth curve γ : $[t_0,t_1] \to Q$ is a *trajectory* of the SOCS (Q,L,C_K,C_V) if

- (1) it satisfies the kinematic constraints: $\gamma^{(2)}(t) \in C_K \ \forall t \in [t_0, t_1]$; and
- (2) it is a critical point of S for the admissible variations: $dS(\gamma)(\delta\gamma) = 0 \ \forall \delta\gamma$ with vanishing end points and such that $\delta\gamma(t) \in C_V|_{\gamma(2)(t)} \ \forall t \in [t_0, t_1]$.

Remark 2.3. All holonomic and nonholonomic systems, *i.e.* constrained systems that satisfy d'Alembert's Principle, can be seen as SOCSs. Indeed, if we have a system (Q, L) with constraints given by a distribution $\mathcal{D} \subset TQ$ (with \mathcal{D} integrable in the holonomic case), defining $C_K := (\tau^{(1,2)})^{-1}(\mathcal{D})$ and $C_V := T^{(2)}Q \times_Q \mathcal{D}$, where $\tau^{(1,2)} : T^{(2)}Q \to TQ$ is the canonical projection, then (Q, L, C_K, C_V) is a SOCS whose dynamics recovers the dynamics of the original system. With the same idea, generalized nonholonomic systems (see [25, 19, 6]) can also be seen as SOCSs.

Systems with (at most) second order constraints satisfying the natural generalization of Chetaev's Principle [10], as those appearing in [23] (with first order Lagrangians, as in [31]), define a particular subclass of SOCSs.

On the other hand, second order vakonomic systems, as considered in [2], are not SOCSs because they are purely variational —that is, their trajectories are critical points of the action restricted to the admissible paths— and they allow Lagrangians that depend on higher order derivatives of the path.

When $C_V|_{\eta}$ is nonempty for all $\eta \in C_K$, and C_V is a submanifold, Theorems 17 and 19 in [7] prove that γ is a trajectory of the system if and only if, $\forall t \in [t_0, t_1]$,

(1)
$$\gamma^{(2)}(t) \in C_K \quad \text{and} \quad D_{EL}L(\gamma^{(2)}(t)) \in F_V|_{\gamma^{(2)}(t)},$$

where $D_{EL}L: T^{(2)}Q \to T^*Q$ is the well known Euler–Lagrange map (see [9], Thm. 2.2.3) and $F_V|_{\eta} := (C_V|_{\eta})^{\circ}$ for all $\eta \in T^{(2)}Q$ is the space of constraint forces. Notice that for nonholonomic systems, given $q \in Q$ and $\eta \in T_q^{(2)}Q$, we have that $F_V|_{\eta} = \mathcal{D}_q^{\circ}$ (see Remark 2.3), that is, the constraint forces vanish on the allowed velocities, which is the content of d'Alembert's Principle.

Under some conditions, it is possible to define the $flow^2 F_L : TQ \times \mathbb{R} \to TQ$ of the system. We are interested in studying the symplecticity of the map $F_L^t : TQ \to TQ$

²In this section we shall ignore issues related to global versus local flows. For SOCSs, there are certain conditions of existence and uniqueness of trajectories when $C_V = (\tau^{(1,2)} \times id_{TQ})^{-1}(C_V')$ for some $C_V' \subset TQ \times_Q TQ$ (see [21], Sect. IV).

corresponding to flowing for a fixed time t. Recall that the Legendre transform of L is $\mathcal{F}L:TQ\to T^*Q$ defined by

$$\mathcal{F}L(v_q)(w_q) := \frac{d}{dz}\bigg|_{z=0} (L(v_q + z \ w_q)), \quad \forall v_q, w_q \in T_q Q.$$

Next, define the Lagrangian 1-form $\theta_L \in \Omega^1(TQ)$ by

$$\theta_L(v_q)(V_{v_q}) := \mathcal{F}L(v_q)(D\tau_Q(v_q)(V_{v_q})), \quad \forall V_{v_q} \in T_{v_q}(TQ),$$

and the Lagrangian 2-form $\Omega_L \in \Omega^2(TQ)$ by

$$\Omega_L := -d\theta_L,$$

which is symplectic for regular Lagrangians. It has been shown in [11] (Sect. 5.1) and in [14] (Sect. II) that, for nonholonomic systems, the symplectic form Ω_L is preserved by the corresponding flow F_L up to an additive exact form. Our next result extends this property to SOCSs and, in particular, to generalized nonholonomic systems.

Theorem 2.4 (Evolution of Ω_L). Let (Q, L, C_K, C_V) be a SOCS with flow F_L : $TQ \times \mathbb{R} \to TQ$ and t be any fixed time. Then,

$$(F_L^t)^*(\Omega_L) = \Omega_L + d\nu,$$

for $\nu \in \Omega^1(TQ)$ defined by

$$\nu(q,\dot{q})(\delta q,\delta \dot{q}) := \int_0^t D_{EL} L(\gamma^{(2)}(s))(\delta q(s)) \ ds, \quad \forall (\delta q,\delta \dot{q}) \in T_{(q,\dot{q})}(TQ),$$

and where γ is the trajectory with initial conditions (q,\dot{q}) and, for $s \in [0,t]$,

$$\delta q(s) := D(\tau_Q \circ F_L^s)(q, \dot{q})(\delta q, \delta \dot{q}) \in T_{\gamma(s)}Q.$$

Proof. The proof is based on [26] (Sect. 1.2.3). Given a smooth curve $\gamma:[0,t]\to Q$ and any variation $\delta\gamma$ of γ (not necessarily with vanishing end points),

$$dS(\gamma)(\delta\gamma) = \int_0^t D_{EL}L(\gamma^{(2)}(s))(\delta\gamma(s)) \ ds + \theta_L(\gamma'(s))(\delta\gamma(s), *)|_0^t,$$

where * is arbitrary but such that $(\delta \gamma(s), *) \in T_{\gamma'(s)}(TQ)$. We define the restricted action functional $\hat{S}: TQ \to \mathbb{R}$ by

$$\hat{S}(q, \dot{q}) := S(\hat{\gamma}),$$

where $\hat{\gamma}$ is the trajectory of the system with initial conditions (q, \dot{q}) . For all $(q, \dot{q}) \in TQ$, and all $(\delta q, \delta \dot{q}) \in T_{(q, \dot{q})}(TQ)$, we define a smooth curve in T(TQ) by $(\delta q(s), \delta \dot{q}(s)) := D(F_L^s)(q, \dot{q})(\delta q, \delta \dot{q})$, whose first component is an infinitesimal variation $\delta \hat{\gamma}$ of $\hat{\gamma}$. We compute

$$d\hat{S}(q,\dot{q})(\delta q,\delta \dot{q}) = dS(\hat{\gamma})(\delta \hat{\gamma})$$

$$= \int_0^t D_{EL}L(\hat{\gamma}^{(2)}(s))(\delta \hat{\gamma}(s)) ds + \theta_L(\hat{\gamma}(s))(\delta q(s),\delta \dot{q}(s))|_0^t,$$

where we have chosen * to be $\delta \dot{q}(s)$ conveniently. Rewriting the second term in the last equality as

$$((F_L^t)^*(\theta_L) - \theta_L)(q, \dot{q})(\delta q, \delta \dot{q}),$$

we find that the 1-form ν of the statement is $d\hat{S} - ((F_L^t)^*(\theta_L) - \theta_L)$, which is well defined on TQ. Finally,

$$d\nu = d\left(d\hat{S} - ((F_L^t)^*(\theta_L) - \theta_L)\right) = d^2\hat{S} - ((F_L^t)^*(d\theta_L) - d\theta_L) = (F_L^t)^*(\Omega_L) - \Omega_L.$$

Remark 2.5. The flow F_L is a symplectomorphism if $d\nu = 0$. When a SOCS is unconstrained, which, in the context of Remark 2.3, means that $\mathcal{D} = TQ$, we have that $D_{EL}L(\gamma^{(2)}(s)) = 0$ in the definition of ν . Hence, in this case, F_L is a symplectomorphism.

In the holonomic case, *i.e.* \mathcal{D} is an integrable distribution, if Σ is an integral submanifold of \mathcal{D} , the flow F_L preserves Σ and is a symplectomorphism with respect to the restriction of Ω_L to it. Indeed, when $(\delta q, \delta \dot{q}) \in T(T\Sigma)$, we have that $\delta q(s)$ remains in $T\Sigma$, so that the term $D_{EL}L(\gamma^{(2)}(s))(\delta q(s))$ in the definition of ν vanishes.

3. Discrete second order constrained Lagrangian systems

Just as SOCSs are an extension of the notion of nonholonomic system, in this section we introduce a discrete time counterpart of SOCSs that is an extension of the notion of discrete nonholonomic system introduced in [11]. Later, in Section 5, we study the existence and uniqueness of trajectories and the symplectic behavior of the discrete time evolution.

Notation: $p_{i,j,\dots}^m$ is the projection on the *i*-th, *j*-th, and so on, variables of Q^m onto Q.

Definition 3.1 (DSOCS). A discrete second order constrained Lagrangian system is a quadruple (Q, L_d, D_K, D_V) where

- (1) Q is as in Definition 2.1,
- (2) $L_d: Q \times Q \to \mathbb{R}$ is a smooth function, the discrete Lagrangian,
- (3) $D_K \subset Q \times Q \times Q$ is a submanifold, the discrete kinematic constraints, and
- (4) $D_V \subset (p_2^3)^*(TQ)$ (where $(p_2^3)^*(TQ)$ is the pullback bundle under p_2^3) is such that for every $(q,q',q'') \in Q^3$ the subset $D_V|_{(q,q',q'')} := D_V \cap (\{(q,q',q'')\} \times T_{q'}Q)$, naturally identified with a subset of $T_{q'}Q$, is a vector subspace, the discrete variational constraints.

The discrete action functional is defined by $S_d(q.) := \sum_{k=0}^{N-1} L_d(q_k, q_{k+1})$ where $q.: \{0, \ldots, N\} \to Q$ is a discrete path in Q. An infinitesimal variation of q. consists of a map $\delta q.: \{0, \ldots, N\} \to TQ$ such that $\delta q_k \in T_{q_k}Q \ \forall k$, and it is said to have vanishing end points if $\delta q_0 = 0$ and $\delta q_N = 0$. The following Principle determines the dynamics of DSOCSs.

Definition 3.2 (Discrete Lagrange–d'Alembert Principle for DSOCSs). A discrete path $q: \{0,\ldots,N\} \to Q$, with $N \geq 2$, is a trajectory of the DSOCS (Q,L_d,D_K,D_V) if

(1) it satisfies the discrete kinematic constraints:

$$(q_{k-1}, q_k, q_{k+1}) \in D_K \quad \forall k \in \{1, \dots, N-1\}, \text{ and }$$

(2) it is a critical point of S_d for the admissible variations: $dS_d(q_{\cdot})(\delta q_{\cdot}) = 0$, $\forall \delta q_{\cdot}$ with vanishing end points and such that

$$\delta q_k \in D_V|_{(q_{k-1}, q_k, q_{k+1})} \quad \forall k \in \{1, \dots, N-1\}.$$

 \neg

Let X be a manifold and X^m its m-th Cartesian product. When $F: X^m \to \mathbb{R}^n$ is a smooth map, its derivative DF is, in a natural way, a differential form on X^m with values in \mathbb{R}^n . On the other hand, if $i_j: (p_j^m)^*(TX) \to T(X^m)$ is the inclusion

$$i_j(\delta x_j) := (0, \dots, 0, \underbrace{\delta x_j}_{j}, 0, \dots, 0),$$

we define

(2)
$$D_j F := i_j^*(DF) = DF \circ i_j.$$

When q is a trajectory of a DSOCS, it follows from the arbitrariness of the admissible variations that, $\forall k \in \{1, ..., N-1\}$,

$$D_1L_d(q_k, q_{k+1}) + D_2L_d(q_{k-1}, q_k) \in (D_V|_{(q_{k-1}, q_k, q_{k+1})})^{\circ}.$$

Inspired by [27] (Prop. 3), we define the section β of D_V^* by

(3)
$$\beta(q_{k-1}, q_k, q_{k+1}) := i_{(q_{k-1}, q_k, q_{k+1})}^t (\mathcal{F}^+ L_d(q_{k-1}, q_k) - \mathcal{F}^- L_d(q_k, q_{k+1})),$$

where the discrete Legendre transforms \mathcal{F}^-L_d and $\mathcal{F}^+L_d: Q \times Q \to T^*Q$ are such that $\mathcal{F}^-L_d(q,q'):=(q,-D_1L_d(q,q'))$ and $\mathcal{F}^+L_d(q,q'):=(q',D_2L_d(q,q'))$ for all $(q,q')\in Q\times Q$, and where $i:D_V|_{\cdot}\hookrightarrow \left(\left(p_2^3\right)^*(TQ)\right)|_{\cdot}$ is the inclusion and i^t_{\cdot} is the transpose map. The following result is straightforward.

Theorem 3.3. A discrete path $q: \{0, ..., N\} \to Q$, with $N \ge 2$, is a trajectory of the DSOCS (Q, L_d, D_K, D_V) if and only if, $\forall k \in \{1, ..., N-1\}$,

(4)
$$(q_{k-1}, q_k, q_{k+1}) \in D_K \quad and \quad \beta(q_{k-1}, q_k, q_{k+1}) = 0.$$

Remark 3.4. A discrete nonholonomic system as introduced in [11] is a discrete Lagrangian system (Q, L_d) with discrete constraint space $\mathcal{D}_d \subset Q \times Q$ (we say first order) and allowed variation distribution $\mathcal{D} \subset TQ$ (we say zeroth order). In particular, a discrete holonomic system, in the sense of Remark 3.3 of [11], corresponds to the case where \mathcal{D} is an integrable distribution and $\mathcal{D}_d = \cup_r \mathcal{N}_r \times \mathcal{N}_r$, where \mathcal{N}_r are the integral submanifolds of \mathcal{D} .

In both cases, their trajectories $q = (q_0, \dots, q_N)$ are the solutions of

$$\begin{cases} D_1 L_d(q_k, q_{k+1}) + D_2 L_d(q_{k-1}, q_k) \in \mathcal{D}_{q_k}^{\circ}, \\ (q_k, q_{k+1}) \in \mathcal{D}_d \end{cases}$$

for all k = 1, ..., N-1 and that, additionally, satisfy $(q_0, q_1) \in \mathcal{D}_d$. Notice that these conditions are equivalent to

$$\begin{cases} D_1 L_d(q_k, q_{k+1}) + D_2 L_d(q_{k-1}, q_k) \in \mathcal{D}_{q_k}^{\circ}, \\ (q_k, q_{k+1}) \in \mathcal{D}_d, \\ (q_{k-1}, q_k) \in \mathcal{D}_d \end{cases}$$

for all k = 1, ..., N-1. In order to ensure the existence of trajectories, it is usually assumed —and we will do so— that the projection $p_1^2: Q \times Q \to Q$ restricted to \mathcal{D}_d is a submersion (see [27], Prop. 3). This last condition is trivially satisfied in the holonomic case.

DSOCSs extend the discrete holonomic and nonholonomic systems as follows. Given a distribution \mathcal{D} and a submanifold \mathcal{D}_d as above, a DSOCS (Q, L_d, D_K, D_V) can be constructed by defining

$$D_K := (Q \times \mathcal{D}_d) \cap (\mathcal{D}_d \times Q)$$
 and $D_V := (p_2^3)^*(\mathcal{D}).$

Notice that D_K is indeed a submanifold of $Q \times Q \times Q$ because it is a transversal intersection of two submanifolds; the transversality condition follows from $p_1^2|_{\mathcal{D}_d}$ being a submersion. It is easy to see that both systems, the discrete nonholonomic system and the related DSOCS, have the same trajectories.

Remark 3.5. Other "higher order" discrete mechanical systems have been considered in the literature. One such example is that of higher order discrete Lagrangian mechanics [1], consisting of unconstrained systems with Lagrangians that may depend on more than two points. Also, discrete higher order vakonomic systems have been considered in, for example, [24]. These are constrained systems where the Lagrangians also depend on more than two points and the trajectories correspond to a purely variational problem, just as in the continuous case mentioned in Remark 2.3.

Remark 3.6. From a theoretical point of view, one could be interested in a discrete analogue of the higher order constrained systems (in the sense of [8, 21]). Such an analogue can be obtained following ideas similar to the ones introduced in this section for order 2. For instance, a discrete kinematic constraint of order k would be a submanifold of Q^{k+1} and the variational constraints of order k would be contained in the pullback bundle by $p_j^{k+1}: Q^{k+1} \to Q$ of TQ for a choice of $j \in \{1, \ldots, k+1\}$.

4. Examples

In this section we discuss how to apply DSOCSs to construct numerical integrators for two (continuous) systems with second order constraints. In each case, we picked simple discretizations to associate a discrete system to the continuous one. Our main objective is to show how the numerical integrator is constructed and some characteristics of its behavior. Other discretizations and details can be found in [4].

In this section, all angles are expressed in radians.

- 4.1. Particle in the plane with prescribed signed curvature. Consider a particle in \mathbb{R}^2 forced to move with a given signed curvature, $k : \mathbb{R}^2 \to \mathbb{R}$, by the effect of a force orthogonal to its velocity. For example, if the particle is electrically charged, this could be achieved using a magnetic field orthogonal to the plane.
- 4.1.1. Continuous case. We first describe the system in terms of Definition 2.1 (see Figure 1 to visualize the meaning of the following variables).
 - (1) $Q := \mathbb{R}^2$, with coordinates q = (x, y).
 - (2) $L((x,y),(\dot{x},\dot{y})):=\frac{1}{2}m(\dot{x}^2+\dot{y}^2)$, where m is the mass of the particle.
 - (3) Kinematic constraints: the submanifold $C_K \subset T^{(2)}Q$ is defined by $\frac{d\theta}{ds} = k(x,y)$, where θ is the polar angle of the velocity of the particle and ds is the element of the arc length. Explicitly, the equation becomes

(5)
$$\frac{\dot{x} \, \ddot{y} - \ddot{x} \, \dot{y}}{\|(\dot{x}, \dot{y})\|^3} = k(x, y).$$

(4) Variational constraints: for each $\eta = ((x, y), (\dot{x}, \dot{y}), (\ddot{x}, \ddot{y})) \in T^{(2)}Q$, the subspace $C_V|_{\eta}$ is defined as the span of (\dot{x}, \dot{y}) in $T_{(x,y)}Q$.

In this case equation (1) is equivalent to equation (5) together with $m\ddot{x} = \lambda \dot{y}$ and $m\ddot{y} = -\lambda \dot{x}$, where λ is an unknown Lagrange multiplier.

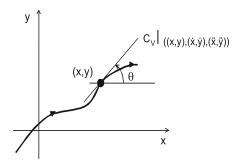


FIGURE 1. Scheme of the particle in the plane with prescribed signed curvature. The polar angle θ of the particle's velocity and the variational constraints at $((x, y), (\dot{x}, \dot{y}), (\ddot{x}, \ddot{y}))$ are indicated

- 4.1.2. Discrete case. We now associate a DSOCS to this SOCS in order to approximate its trajectory q(t) by a discrete one, q, in such a way that $q_0 \approx q(0)$, $q_1 \approx q(h)$, $q_2 \approx q(2h)$, and so on, where $h \in \mathbb{R}$ is the constant time step. We use the following particular discretization process.
 - (1) $Q = \mathbb{R}^2$
 - (2) $L_d := L \circ \varphi_{L_d}^{-1}$ where $\varphi_{L_d} : TQ \to Q^2$ is defined in terms of its inverse by

$$\varphi_{L_d}^{-1}(q_0, q_1) := \left(q_0, \frac{q_1 - q_0}{h}\right).$$

(3) Discrete kinematic constraints: $D_K := \varphi_{D_K}(C_K)$ where $\varphi_{D_K}: T^{(2)}Q \to Q^3$ is defined by

$$\varphi_{D_K}^{-1}(q_0, q_1, q_2) := \left(q_1, \frac{q_2 - q_0}{2h}, \frac{q_2 - 2q_1 + q_0}{h^2}\right).$$

(4) Discrete variational constraints: defining $\varphi_{D_V} := \varphi_{D_K}$,

$$\begin{split} D_V|_{(q_0,q_1,q_2)} &:= C_V|_{\varphi_{D_V}^{-1}(q_0,q_1,q_2)} \\ &= \left\langle \left\{ \left((x_1,y_1), \frac{x_2 - x_0}{2h} \ \frac{\partial}{\partial x_1} + \frac{y_2 - y_0}{2h} \ \frac{\partial}{\partial y_1} \right) \right\} \right\rangle. \end{split}$$

Equation (4) leads to a system of nonlinear equations in x_2 and y_2 ,

(6)
$$\frac{\frac{x_2 - x_0}{2h} \frac{y_2 - 2y_1 + y_0}{h^2} - \frac{x_2 - 2x_1 + x_0}{h^2} \frac{y_2 - y_0}{2h}}{\left\| \left(\frac{x_2 - x_0}{2h}, \frac{y_2 - y_0}{2h} \right) \right\|^3} = k(x_1, y_1)$$

(7)
$$(x_2 - 2x_1 + x_0)(x_2 - x_0) + (y_2 - 2y_1 + y_0)(y_2 - y_0) = 0.$$

To simulate the case for which k=1, x(0)=y(0)=0 and $\dot{x}(0)=\dot{y}(0)=1$, we took different values of h and solved equations (6) and (7) iteratively (using the algorithm FindRoot of Mathematica 6.0 at each step) starting with the discrete initial conditions $x_0=y_0=0$, $x_1=x_0+h$ and $y_1=y_0+h$. In this situation, we know that the exact solutions of the continuous equations of motion are

$$x(t) = \cos(\sqrt{2}t - \frac{\pi}{4}) - \frac{\sqrt{2}}{2}$$
 and $y(t) = \sin(\sqrt{2}t - \frac{\pi}{4}) + \frac{\sqrt{2}}{2}$.

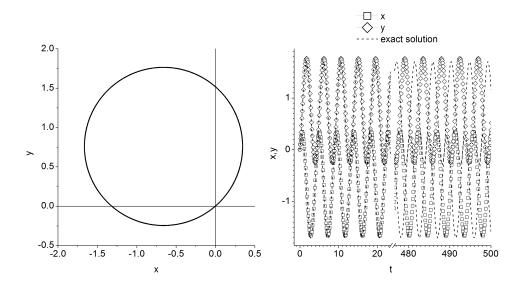


FIGURE 2. Simulated evolution of the particle using our numerical integrator constructed from a DSOCS for k=1, x(t)=y(t)=0 and $\dot{x}(0)=\dot{y}(0)=1$. Constant time step used: h=0.1. LEFT: trajectory on the plane, RIGHT: comparison between our approximation and the exact solutions of x and y over two time intervals

On the one hand, we found our results satisfactory at a qualitative level (see Figure 2 corresponding to h=0.1): as expected, the trajectory in the plane is a circumference of radius 1 which passes through the origin and is tangent to the line of slope 1 at that point; there are no changes in the amplitude and the frequency of the oscillations of x and y during the time of simulation [0,500]. This good behavior may be partially due to the following property of the system: since each summand in equation (7) is a difference of squares, $(x_2-x_1)^2-(x_1-x_0)^2+(y_2-y_1)^2-(y_1-y_0)^2$ equals zero, so we have that $L_d(q_0,q_1)=L_d(q_1,q_2)$, i.e. our numerical integrator preserves the (discretized) energy of the system as it occurs in the continuous case. Apart from that, we can also say our integrator is symmetric [22].

On the other hand, on the right side of Figure 2 we see how the simulated evolution is slowly left behind by the exact solution. Their maximum difference occurs near t=500. This maximum difference over the [0,500] time interval is what we take for the error of the numerical integrator. Figure 3 shows the error for several values of the time step h. The slope of the line shown in the graph (≈ 1.6) suggests that the integrator is convergent of order 1, according to Section 2.2.2 of [26].

4.2. Inertia wheel pendulum with a Lyapunov constraint. In Reference [20], a method for asymptotic stabilization of underactuated mechanical systems has been studied. It consists of: (1) impose on the system a second order constraint of the form

(8)
$$\frac{dV}{dt}(q(t), \dot{q}(t)) = -F(q(t), \dot{q}(t)),$$

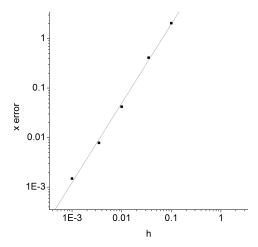


Figure 3. Plot of the x-coordinate error vs h, using logarithmic scales

the so-called Lyapunov constraints, where $F,V:TQ\to\mathbb{R}$ are nonnegative functions with V proper and vanishing only at the desired equilibrium point; and (2) find the related constraint force (to be implemented by the actuators), which would play the role of the control law. It is clear that, if the system satisfies the previous constraints, then $V(q(t),\dot{q}(t))$ decreases over time, resulting in a Lyapunov function. In order to ensure the existence of a related constraint force, V must satisfy a PDE that depends on the actuators.

It can be shown, in general, that the underactuated system (*i.e.* the mechanical system and the actuators) together with the Lyapunov constraint define a SOCS. In the case of the inertia wheel pendulum with one actuator on the wheel (see Figure 4), if we want to asymptotically stabilize it at the upright position, we can

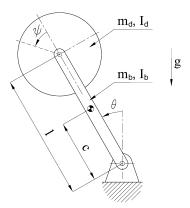


FIGURE 4. Scheme of the inertia wheel pendulum. Some of the physical parameters associated to its components (masses, lengths and moments of inertia) as well as the coordinates used are indicated

use the functions V and F found in [20] (Sect. 5.1). The SOCS defined by the inertia wheel pendulum and the mentioned Lyapunov constraint is described below.

- 4.2.1. Continuous case. We start by adapting the Hamiltonian description of the system given in [20] to the variational formulation of SOCSs.
 - (1) $Q := S^1 \times S^1$, with coordinates $q = (\theta, \psi)$.
 - (2) $L(\theta, \psi, \dot{\theta}, \dot{\psi}) := \frac{1}{2}I\dot{\theta}^2 + \frac{1}{2}J(\dot{\theta} + \dot{\psi})^2 Mg(1 + \cos(\theta))$, where g is the acceleration of gravity and I, J and \tilde{M} are defined in terms of the masses, moments of inertia and characteristic lengths of the components of the system by $I := m_b c^2 + m_d l^2 + I_b$, $J := I_d$ and $\tilde{M} := m_b c + m_d l$.
 - (3) Kinematic constraints: the submanifold $C_K \subset T^{(2)}Q$ is defined by equation (8) by choosing³

$$\begin{split} V(\theta, \psi, \dot{\theta}, \dot{\psi}) &:= \frac{1}{2} f[(I+J)\dot{\theta} + J\dot{\psi}]^2 \\ &+ \frac{1}{2} h_c J^2 (\dot{\theta} + \dot{\psi})^2 + g_c J[(I+J)\dot{\theta} + J\dot{\psi}] (\dot{\theta} + \dot{\psi}) \\ &+ \chi [1 - \cos(\psi - n\theta)] + \frac{Me}{d} (1 - \cos(\theta)), \\ F(\theta, \psi, \dot{\theta}, \dot{\psi}) &:= \rho \ \tanh\{g_c [(I+J)\dot{\theta} + J\dot{\psi}] + h_c J(\dot{\theta} + \dot{\psi})\} \\ &\cdot \{g_c [(I+J)\dot{\theta} + J\dot{\psi}] + h_c J(\dot{\theta} + \dot{\psi})\}, \end{split}$$

where $\chi, \rho, d, e > 0$, $M := \tilde{M}g$, $h_c := d\frac{nb-c}{ac-b^2}$, $g_c := d\frac{na-b}{ac-b^2}$, $f := \frac{g_c^2 + e}{h_c}$ with $a := \frac{1}{I}$, $b := -\frac{1}{I}$, $c := \frac{1}{I} + \frac{1}{J}$, and $n \in \mathbb{Z}$ is such that nb > c. Note that (8) becomes a second order differential equation.

(4) Variational constraints: for $\eta = ((\theta, \psi), (\dot{\theta}, \dot{\psi}), (\ddot{\theta}, \ddot{\psi})) \in T^{(2)}Q$, the subspace $C_V|_{\eta}$ is defined as the span of $\frac{\partial}{\partial \theta}|_{(\theta,\psi)}$ in $T_{(\theta,\psi)}Q$.

Then, the trajectory conditions (1) become (8) and the system $\tilde{M}g \sin(\theta) - I\ddot{\theta}$ $J(\ddot{\theta} + \ddot{\psi}) = 0$, $-J(\ddot{\theta} + \ddot{\psi}) = \lambda$, where λ is an unknown lagrange multiplier.

- 4.2.2. Discrete case. We want to construct a numerical integrator of the equations of motion of this SOCS to provide an approximation of q(t) as in Section 4.1.2. From now on, we replace $S^1 \times S^1$ with its universal covering space \mathbb{R}^2 and adapt all the elements of our SOCS to this new configuration space, which can be done easily by letting (θ, ψ) vary over all the plane. Physically, we capture the same dynamics by doing so but, for practical issues, this allows us to discretize the whole TQ space by using a diffeomorphism onto $Q \times Q$. Recalling the discretizations φ_{L_d} and φ_{D_K} used in Section 4.1.2, we propose the following DSOCS:
 - (1) $Q := \mathbb{R}^2$.

 - (2) $L_d := L \circ \varphi_{L_d}^{-1}$. (3) Discrete kinematic constraints: $D_K := \varphi_{D_K}(C_K)$.
 - (4) Discrete variational constraints: $D_V|_{(q_0,q_1,q_2)} := C_V|_{\varphi_{D_V}^{-1}(q_0,q_1,q_2)}$.

The second condition of (4) leads to

(9)
$$(I+J)\frac{(\theta_2 - 2\theta_1 + \theta_0)}{h^2} + J\frac{(\psi_2 - 2\psi_1 + \psi_0)}{h^2} - M\sin(\theta_1) = 0.$$

 $^{^3}$ The choices, explained in detail in [20], are aimed at making V an energy-like function and F a bounded function satisfying certain relations to guarantee the realization of the system as an actuated system under a bounded control signal.

Substituting ψ_2 from (9) into the first condition of (4) leads to a nonlinear equation involving only θ_2 ,

(10)
$$A\theta_2^2 + B\theta_2 + C = -\rho \tanh(D\theta_2 + E)(D\theta_2 + E),$$

where A equals the constant $-\frac{dI^2(I+(n+1)J)}{2h^3}$, and B, C, D and E depend on the system constants, the time step h, and the initial data θ_0 , θ_1 , ψ_0 and ψ_1 .

We used this DSOCS as a numerical integrator and tested it with parameters $I=312.5,\ J=2.0772,\ M=37.98,\ d=1,\ e=1000,\ \chi=100,\ n=-154,$ $\rho=2,$ and initial conditions $\theta(0)=0.5,\ \psi(0)=0,\ \dot{\theta}(0)=0,\ \dot{\psi}(0)=0.5.$ We took different values of h and solved (10) iteratively (using the algorithm FindRoot of Mathematica 6.0 and then calculating ψ_2 using (9)) starting with the discrete initial conditions $\theta_0=0.5,\ \psi_0=0,\ \theta_1=\theta_0$ and $\psi_1=\psi_0+0.5h$.

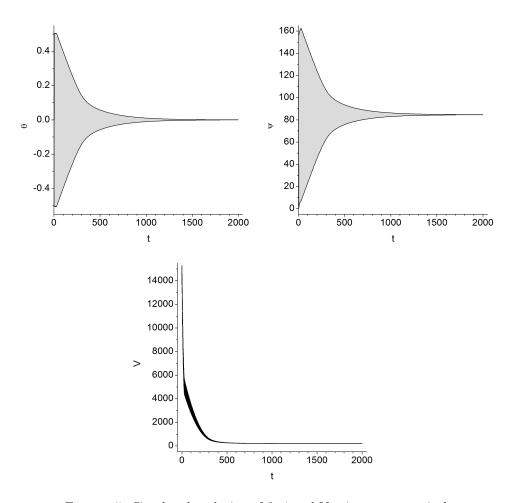


FIGURE 5. Simulated evolution of θ , ψ and V using our numerical integrator constructed from a DSOCS for the initial conditions $\theta(0) = 0.5$, $\psi(0) = 0$, $\dot{\theta}(0) = 0$, $\dot{\psi}(0) = 0.5$. Constant time step used: h = 0.1. The gray area in the first two graphs corresponds to a fast oscillation

Solutions of equation (10), whenever they exist, usually come in pairs, but in order to simulate the evolution of our SOCS we had to choose one. This phenomenon is a consequence of the equations of motion being algebraic equations —rather than differential equations—and, so, it is present in all types of discrete mechanical systems, including DSOCSs. For the present example, we adopted the criterion of picking the solution that is closer to the previous position θ in each step. However, this works as long as the two candidate solutions are sufficiently apart. When this does not occur, we noticed that the correct behavior is obtained by choosing the solution that decreases F and, consequently V, as desired.

To test the behavior of our numerical integrator, we used the output of the sophisticated algorithm NDSolve of Mathematica 6.0 as the exact solution. Figure 5 corresponds to a time step h=0.1; the plots obtained with NDSolve are omitted in there because they are indistinguishable from those coming from our simulations, at least, for the scales used in the figure. Hence, our simulations are consistent qualitatively with the one provided by NDSolve. The coordinates θ and ψ exhibit damped oscillatory behavior in time associated to the asymptotic stabilization of the pendulum at its upright position ($t \approx 1000$); as it is required by the kinematic constraint, the value of the Lyapunov function decreases with time tending to zero ($t \approx 500$).

As in the previous example, we use the maximum difference between the numerical integrator and NDSolve solutions over the [0,2000] time interval as the error of the numerical integrator. Figure 6 shows the error for several values of the time step h. The slope of the line shown in the graph (≈ 1.3) suggests that the integrator is convergent of order 1, according to Section 2.2.2 of [26].

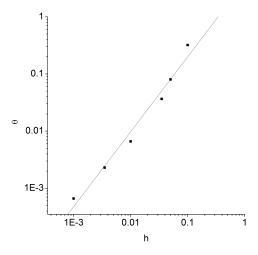


FIGURE 6. Plot of the θ -coordinate error vs h, using logarithmic scales

5. Some properties of the discrete flow

In this section we study the evolution of a DSOCS from the point of view of a discrete flow function. Let (Q, L_d, D_K, D_V) be a DSOCS such that D_V is a vector subbundle of $(p_2^3)^*(TQ)$. Fix a trajectory (q_0, q_1, q_2) of the system and an

open set $U \subset Q \times Q \times Q$ containing it. It is convenient to choose a smooth map $\phi: D_V^*|_U \to \mathbb{R}^{n_V}$ such that $\phi^{-1}(\{0\})$ is the image of the zero section of $D_V^*|_U$ (locally, this imposes no restriction). Then, we have the following existence result.

Theorem 5.1 (Discrete flow). Assume that the DSOCS described above also satisfies the following conditions.

- (1) $\phi \circ \beta|_{D_K \cap U}$ has constant rank,
- (2) The restrictions of $D_3(\phi \circ \beta|_U)(q_0, q_1, q_2)$ and $D_1(\phi \circ \beta|_U)(q_0, q_1, q_2)$ to the subspace $T_{(q_0, q_1, q_2)}D_K$ are injective (see (2)).

Then, there exists a diffeomorphism $F_{L_d}: C_d \to F_{L_d}(C_d)$, called discrete flow, between submanifolds of $Q \times Q$ containing (q_0, q_1) and (q_1, q_2) , respectively, such that

i.
$$F_{L_d}(q_0, q_1) = (q_1, q_2)$$
 and
ii. $(\hat{q}_0, \hat{q}_1, (p_2^2 \circ F_{L_d})(\hat{q}_0, \hat{q}_1))$ is a trajectory $\forall (\hat{q}_0, \hat{q}_1) \in C_d$.

Proof. Section β defined in (3) is smooth due to the smoothness of D_V . From condition 1 in the statement, $W:=(\phi\circ\beta|_{D_K\cap U})^{-1}(\{0\})$ is a submanifold of $D_K\cap U$. All the elements of W are trajectories since they are the triples which satisfy condition (4). On the other hand, as $\ker(Dp_{1,2}^3|_W(q_0,q_1,q_2))=\ker(D(\phi\circ\beta|_{D_K\cap U})(q_0,q_1,q_2))\cap T_{(q_0,q_1,q_2)}(\{q_0\}\times\{q_1\}\times Q)$, which vanishes by condition 2 in the statement, $p_{1,2}^3|_W$ is a local diffeomorphism between a neighborhood $B\subset W$ of (q_0,q_1,q_2) and a submanifold of $Q\times Q$ containing (q_0,q_1) . Analogously, by condition 2 in the statement, $p_{2,3}^3|_W$ is a local diffeomorphism between a neighborhood $B'\subset W$ of (q_0,q_1,q_2) and a submanifold of $Q\times Q$ containing (q_1,q_2) . Finally, let $C_d:=p_{1,2}^3(B\cap B')$ and define

$$F_{L_d}: C_d \to Q \times Q \quad \text{ by } \quad F_{L_d}:=p_{2,3}^3 \circ (p_{1,2}^3|_{B \cap B'})^{-1}.$$

Then C_d and $F_{L_d}(C_d) = p_{2,3}^3(B \cap B')$ are submanifolds of $Q \times Q$, $F_{L_d} : C_d \to F_{L_d}(C_d)$ is a diffeomorphism and conditions i and ii in the statement are satisfied.

Remark 5.2. When a DSOCS comes from a discrete holonomic system (see Remark 3.4), we have that

$$C_d \subset p_{1,2}^3(D_K) \subset \mathcal{D}_d = \cup_r \mathcal{N}_r \times \mathcal{N}_r.$$

Let $C_{d,r} := C_d \cap (\mathcal{N}_r \times \mathcal{N}_r)$. It is easy to check that $F_{L_d}(C_{d,r}) = F_{L_d}(C_d) \cap (\mathcal{N}_r \times \mathcal{N}_r)$.

Let Q and L_d be as in Definition 3.1. Following the literature (see [11]), we define the discrete Lagrangian 1-forms $\theta_{L_d}^-$, $\theta_{L_d}^+ \in \Omega^1(Q \times Q)$ by

(11)
$$\theta_{L_d}^-(q, q')(v_q, v_{q'}) := \mathcal{F}^- L_d(q, q')(v_q) \\ \theta_{L_d}^+(q, q')(v_q, v_{q'}) := \mathcal{F}^+ L_d(q, q')(v_{q'})$$

for all $(v_q, v_{q'}) \in T_{(q,q')}(Q \times Q)$. In addition, we define the discrete Lagrangian 2-form $\Omega_{L_d} \in \Omega^2(Q \times Q)$ as $\Omega_{L_d} := -d\theta_{L_d}^+ = -d\theta_{L_d}^-$ (the last equality is true because $dL_d = \theta_{L_d}^+ - \theta_{L_d}^-$). It can be seen that, under certain conditions of regularity on L_d , Ω_{L_d} is a symplectic form.

Theorem 5.3 (Evolution of Ω_{L_d}). Let (Q, L_d, D_K, D_V) be a DSOCS with discrete flow $F_{L_d}: C_d \to F_{L_d}(C_d)$. Also, let $\Omega_{L_d}^{C_d} \in \Omega^2(C_d)$ and $\Omega_{L_d}^{F_{L_d}(C_d)} \in \Omega^2(F_{L_d}(C_d))$ be the restrictions of Ω_{L_d} to the corresponding submanifolds of $Q \times Q$. Then,

$$(F_{L_d})^* \left(\Omega_{L_d}^{F_{L_d}(C_d)}\right) = \Omega_{L_d}^{C_d} + d\xi,$$

where $\xi \in \Omega^1(C_d)$ is defined by

(12)
$$\xi(q_0, q_1)(\delta q_0, \delta q_1) := (\mathcal{F}^+ L_d(q_0, q_1) - \mathcal{F}^- L_d(F_{L_d}(q_0, q_1)))(\delta q_1)$$
 for all $(q_0, q_1) \in C_d$, and all $(\delta q_0, \delta q_1) \in T_{(q_0, q_1)} C_d$.

Proof. The proof is based on [26] (Sect. 1.3.2). Let $(q_0, q_1) \in C_d$ and $(\delta q_0, \delta q_1) \in T_{(q_0, q_1)}C_d$. If $q_2 := (p_2^2 \circ F_{L_d})(q_0, q_1)$ we can interpret $(\delta q_0, \delta q_1)$ as an infinitesimal variation of the initial condition inducing the infinitesimal variation $\delta q_2 := D(p_2^2 \circ F_{L_d})(q_0, q_1)(\delta q_0, \delta q_1)$ over q_2 . Define the restricted discrete action functional $\hat{S}_d : C_d \to \mathbb{R}$ by

$$\hat{S}_d(q_0, q_1) := S_d(q_0, q_1, (p_2^2 \circ F_{L_d})(q_0, q_1)).$$

From the definitions of the Lagrangian 1-forms (11) it is easy to see that

$$\begin{split} d\hat{S}_{d}(q_{0},q_{1})(\delta q_{0},\delta q_{1}) &= dS_{d}(q_{0},q_{1},q_{2})(\delta q_{0},\delta q_{1},D(p_{2}^{2}\circ F_{L_{d}})(q_{0},q_{1})(\delta q_{0},\delta q_{1})) \\ &= (\mathcal{F}^{+}L_{d}(q_{0},q_{1})-\mathcal{F}^{-}L_{d}(q_{1},(p_{2}^{2}\circ F_{L_{d}})(q_{0},q_{1})))(\delta q_{1}) \\ &+ \left[\theta_{L_{d}}^{+}(q_{1},q_{2})(\delta q_{1},\delta q_{2})-\theta_{L_{d}}^{-}(q_{0},q_{1})(\delta q_{0},\delta q_{1})\right]. \end{split}$$

The bracketed term in the last sum is

$$(F_{L_d}^*((\theta_{L_d}^+)^{F_{L_d}(C_d)}) - (\theta_{L_d}^-)^{C_d})(q_0, q_1)(\delta q_0, \delta q_1),$$

where $(\theta_{L_d}^-)^{C_d}$ and $(\theta_{L_d}^+)^{F_{L_d}(C_d)}$ are the restrictions of $\theta_{L_d}^-$ and $\theta_{L_d}^+$ to $\Omega^2(C_d)$ and $\Omega^2(F_{L_d}(C_d))$, respectively. Since (q_0,q_1) and $(\delta q_0,\delta q_1)$ are arbitrary, using (12) we obtain

$$\xi = d\hat{S}_d - (F_{L_d}^*((\theta_{L_d}^+)^{F_{L_d}(C_d)}) - (\theta_{L_d}^-)^{C_d}).$$

Therefore,

$$\begin{split} d\xi &= d(d\hat{S}_d - (F_{L_d}^*((\theta_{L_d}^+)^{F_{L_d}(C_d)}) - (\theta_{L_d}^-)^{C_d})) \\ &= d^2\hat{S}_d + F_{L_d}^*(-d(\theta_{L_d}^+)^{F_{L_d}(C_d)}) - (-d(\theta_{L_d}^-)^{C_d}) \\ &= F_{L_d}^*(\Omega_{L_d}^{F_{L_d}(C_d)}) - \Omega_{L_d}^{C_d}. \end{split}$$

Remark 5.4. The flow F_{L_d} is a symplectomorphism if $d\xi=0$. It follows from (12) that ξ vanishes when $\delta q_1 \in D_V|_{(q_0,q_1,F_{L_d}(q_0,q_1))}$. This situation occurs, for instance, when a DSOCS comes from an unconstrained system, where $D_V|_{(q_0,q_1,F_{L_d}(q_0,q_1))}=T_{q_1}Q$. It also occurs when it comes from a discrete holonomic system (see Remark 3.4). Indeed if $(q_0,q_1) \in C_{d,r}$ (see Remark 5.2) and $(\delta q_0,\delta q_1) \in T_{(q_0,q_1)}C_{d,r}$, we have that $\delta q_1 \in T_{q_1}\mathcal{N}_r = D_V|_{(q_0,q_1,F_{L_d}(q_0,q_1))}$, so that $\xi(q_0,q_1)(\delta q_0,\delta q_1)=0$. Hence, under these conditions,

$$(F_{L_d}|_{C_{d,r}})^* \left(\Omega_{L_d}^{F_{L_d}(C_{d,r})}\right) = \Omega_{L_d}^{C_{d,r}},$$

so that $F_{L_d}|_{C_{d,r}}$ is a symplectomorphism.

6. Future work

It is well known that systems with group symmetry can be reduced and the resulting systems provide a useful way to understand the "core" dynamics and, in some cases, a practical way of solving their equations of motion. Therefore, it is a very natural continuation of the current work to introduce a notion of DSOCS with symmetry group and develop a reduction procedure for these systems. We intend to tackle this problem following the approach to reduce discrete nonholonomic systems used in [17].

Given a numerical integrator of a continuous system, it is very important to know how well it approximates the actual solution of the original system. In the unconstrained case, such analysis can be performed as follows. As a first step, an exact discrete Lagrangian is defined: it has the property that its discrete trajectories coincide with the trajectories of the original system (at specific discrete times). Except in a few trivial cases, such exact Lagrangians cannot be constructed explicitly, so a second step is to construct discrete Lagrangians that approximate the exact one. Using this approach, it is possible to give estimates of the goodness of the numerical integrator (see [26], Part 2). For discrete systems with nonholonomic constraints the same type of error analysis was started in [14]. However, their work still needs to be completed after the results of [29]. Perhaps, this could be done by giving an adequate extension of [29] to the nonholonomic case. Even more, we would like to extend the whole program to the error analysis of DSOCSs.

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E-mail address: bordan@ib.cnea.gov.ar
E-mail address: jfernand@ib.edu.ar
E-mail address: sergiog@cab.cnea.gov.ar