XLI CILAMCE
XLI Ibero-Latin American Congress on Computational Methods in Engineering
16-19 November, 2020 FOZ DO IGUAÇU PARANÁ - BRAZIL

A comparison of geometric integrators for nonconservative and nonholonomic systems

Elias Maciel[1], Inocencio Ortiz[1], Christian E. Schaerer[1]

[1]*Polytechnic School, National University of Asuncion*
Campus Universitario, P.O. Box: 2111 SL, San Lorenzo, Paraguay
emaciel@pol.una.py, inortiz08@gmail.com, cschaer@pol.una.py

Abstract. In this paper, we incorporate nonholonomic constraints to the contact integrator obtained from the Herglotz' variational principle. This results in a geometric integrator which is suitable for nonconservative, nonholonomic systems. We compare this integrator with the more traditional one obtained from the Lagrange-d'Alembert principle. The comparison is performed using numerical simulations on both holonomic and nonholonomic cases. For the holonomic case, in addition to the numerical simulations we present a recently developed backward error analysis.

Keywords: geometric integrator, contact integrator, nonholonomic constraint, nonconservative systems

1 Introduction

Geometric integrators are numerical methods compatible with the underlying geometry of mechanical systems. As a consequence, they have good conservation properties in long-time simulations [1]. Variational mechanics allows systematic ways to get geometric integrators, by discretizing the relevant variational principle [2].

In this context, the case of conservative holonomically constrained systems is the best understood, namely: the configuration space is a manifold Q, the dynamics is encoded in the Lagrangian $L\colon TQ \to \mathbb{R}$ on the tangent bundle of Q, the geometric framework symplectic geometry, and the equations of motion are given by Hamilton's principle of stationary action [3, 4]. Moreover, discretizing Hamilton's principle one gets geometric integrators which preserve the symplectic structure, and as a consequence, they display good conservation features for long-time simulations [2].

For nonconservative holonomically constrained systems there is no such a unified geometric and variational description. However, many interesting systems, such as those subject to Rayleigh dissipation, fall into the following framework: the configuration space is a manifold Q, the Lagrangian is a function $L\colon TQ \times \mathbb{R} \to \mathbb{R}; L = L(q, \dot{q}, z)$, the geometric framework is contact geometry, and the equations of motion are derived from Herglotz' variational principle [5–8]. Moreover, as it was shown in the recent work [9], the discretization of Herglotz' principle yields geometric integrators preserving the contact structure.

The situation regarding constraints is more subtle. The most traditional way to approach nonholonomic systems in a variational framework is based on Lagrange-d'Alembert (LA) principle, which provides the right equations of motion, although it is not a fully variational formulation [10]. By discretizing the LA principle and the constraints in a compatible way, in [11] the authors derived a geometric integrator which falls in the category of *nonholonomic integrators*. By numerical experiments, these integrators are shown to have interesting conservation properties. However, the fundamental reason why nonholonomic integrators in general display good behavior is subtle [12].

Since the fundamental variational principle behind nonconservative systems is Herglotz' principle, it is expected that an integrator for a nonconservative, nonholonomic system obtained by this principle should display better performance than the one coming from LA principle. In a more recent work, the case of nonconservative, nonholonomic systems was studied in the framework of Herglotz' variational principle [5], lying the foundation for a systematic approach in getting contact nonholonomic integrators.

In this work we bring together ideas from the aforementioned works in order to construct a geometric integrator for a nonconservative nonholonomically constrained system, by discretizing its underlying Herglotz' variational principle and the nonholonomic constraints following the same criterion of compatibility considered in [11]. To

compare the integrator obtained from Herglotz' principle with the one obtained from the LA principle, we consider two scenarios: for the case of holonomic systems we perform a backward error analysis, as well as numerical simulations, taking the damped harmonic oscillator as benchmark. For the nonholonomic case, we perform a numerical simulations taking the damped Foucault pendulum as benchmark. We note that a backward error analysis for nonholonomically constrained systems is left for future work.

The structure of this article is as follows. In Section 2 we briefly review the variational principles of interest to us, namely the Lagrange-d'Alembert principle and the Herglotz principle, as well as their their discretization, and explain how we incorporate nonholonomic constraints to the discrete Herglotz principle. In Section 3 we present the simulated mechanical systems and derive their respective Lagrangians to perform qualitative and quantitative comparisons of the presented integrators. Finally, in Section 4 we give some general conclusions and point some lines for future work.

2 Theoretical background

In this section we briefly recall the variational integration paradigm, concentrating in the two variational principles of interest to us, namely, the Lagrange-d'Alembert principle and the Herglotz principle, summarizing the integrators coming from them. Following that, we describe how to incorporate nonholonomic constraints to the integrator coming from Herglotz' principle.

2.1 Discrete variational principles

If $L = L(q, \dot{q})$ is the Lagrangian of a mechanical system with configuration space Q, subject to external forces F^e, the Lagrange-d'Alembert principle states that the path $q\colon [a,b] \to Q$ followed by the system satisfies $\delta \int_a^b L(q,\dot{q})\,\mathrm{d}t + \int_a^b F^e \cdot \delta q\,\mathrm{d}t = 0$. If the system is subject to constraints $D \subset TQ$ (given locally by the vanishing of m functions $\{\Phi^c\}_{c=1}^m$, linear in the velocities), the variations δq are asked to satisfy these constraints. This leads to the usual forced Euler-Lagrange (EL) equations with Lagrange multipliers [10]. The point with variational integrators is not to go to the EL equations, but instead, to discretize the variational principle itself (and the constraints), which, in this case, yields the following forced constrained *Discrete Euler-Lagrange equations*:

$$\begin{aligned} D_1 L_d(q_j, q_{j+1}) + D_2 L_d(q_{j-1}, q_j) + F_d^+(q_{j-1}, q_j) + F_d^-(q_j, q_{j+1}) &= \lambda_c \Phi^c, \\ \Phi_d^c(q_j, q_{j+1}) &= 0, \end{aligned} \tag{1}$$

where $L_d\colon Q \times Q \to \mathbb{R}$ is the *discrete Lagrangian* ($L_d(q_j, q_{j+1}) \simeq \int_{t_j}^{t_{j+1}} L(q,\dot{q})\,\mathrm{d}t$), $F_d^\pm$ are the *discrete forces*, Φ_d^c are the *discrete constraints* and λ_c are Lagrange multipliers (see [2] and [11] for details). D_i indicates the partial derivative with respect to the i-th argument.

For a forced system, the Herglotz variational principle consider a Lagrangian $L\colon TQ \times \mathbb{R} \to \mathbb{R}$, $L = L(q,\dot{q},z)$, and states that the path $q\colon [a,b] \to Q$ followed by the systems are those who are critical points of the action $z(b)$, where $z\colon [a,b] \to \mathbb{R}$ is a solution of the initial value problem $\dot{z} = L(q,\dot{q},z)$ with $z(a) = 0$. This is equivalent to the path $q(t)$ being a solution of the *Herglotz equations* (or *generalized Euler-Lagrange equations*):

$$\frac{\partial L}{\partial q^i} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}^i} + \frac{\partial L}{\partial \dot{q}^i}\frac{\partial L}{\partial z} = 0. \tag{2}$$

Following the paradigm of variational integration, instead of discretizing the Hetglotz equations, one can discretize Herglotz' principle to get the *discrete Herglotz equations*:

$$D_1 L_d(q_j, q_{j+1}, z_j, z_{j+1}) + D_2 L_d(q_{j-1}, q_j, z_{j-1}, z_j)\frac{1 + hD_3 L_d(q_j, q_{j+1}, z_j, z_{j+1})}{1 - hD_4 L_d(q_{j-1}, q_j, z_{j-1}, z_j)} = 0, \tag{3}$$

which yields an integrator $(q_{j-1}, q_j) \mapsto (q_j, q_{j+1})$, provided some usual nondegeneracy condition holds. This integrator preserves the natural contact structure associated to the Lagrangian L_d [9].

Remark 1 (Backward error analysis)**.** *Backward error analysis for variational integrators seeks for modified Lagrangians which are exactly solved by the integrator coming from the discretization of the variational principle. The cases of LA principle and Herglotz' principle, both for holonomic systems, were recently investigated in [13] and [9]. In this work we merely intend to apply the results obtained there.*

2.2 Contact nonholonomic integrator

Now consider that the system described by the Lagrangian $L\colon TQ \times \mathbb{R} \to \mathbb{R}$, together with Herglotz' principle, is subject to a constraint $D \subset TQ$ described locally by the functions $\{\Phi^c\}_{c=1}^m$. Following ideas from [11], in order to get our contact nonholonomic integrator, we consider a *discrete constraint*, given by a submanifold $D_d \subset Q \times Q$, such that $(q,q) \in D_d$, for all $q \in Q$. This submanifold imposes a constraint on the discrete curves $(q_0, q_1, \ldots, q_N)$, in the sense that we must have $(q_j, q_{j+1}) \in D_d$. Now we consider the discrete Herglotz principle, but allowing only variations of the discrete curve (q_j), with fixed endpoints q_0, q_N, and satisfying the (continuous) constraint, namely, $\delta q_j \in D_{q_j}$. By doing so, we get that the discrete curves (q_j) satisfying the constrained discrete Herglotz principle are those satisfying the following equations (in terms of Lagrange multipliers λ_c):

$$\begin{aligned} D_1L_d(q_j,q_{j+1},z_j,z_{j+1}) + D_2L_d(q_{j-1},q_j,z_{j-1},z_j)\frac{1+hD_3L_d(q_j,q_{j+1},z_j,z_{j+1})}{1-hD_4L_d(q_{j-1},q_j,z_{j-1},z_j)} &= \lambda_c\Phi^c, \\ \Phi^c_d(q_j,q_{j+1}) &= 0. \end{aligned} \tag{4}$$

The most natural way to choose the discrete constraint D_d is by considering its defining functions Φ^c_d to be a discretization of the continuous functions Φ^c defining the continuous constraint D. Following [11], we may consider a discretizing map $\Psi\colon Q\times Q \to TQ$ such that $L_d = L\circ\Psi$, and then, take $\Phi^c_d = \Phi^c\circ\Psi$. Equation (4) thus provides, under usual regularity condition, an integrator $(q_{j-1},q_j) \mapsto (q_j,q_{j+1})$, respecting the discrete constraint.

3 Experimental settings and numerical results

In this section we describe the two mechanical systems we are going to use as benchmark to test the integrators, namely: the damped harmonic oscillator and the damped Foucault pendulum.

3.1 Damped harmonic oscillator

This system consists of a harmonic oscillator with mass m that undergoes a Rayleigh dissipation, i.e. a dissipation force proportional to the velocities with parameter α. For simplicity, in all the applications we consider $m = 1$.

Lagrange-d'Alembert description: In this context, the Lagrangian for this system is

$$L(q,\dot q) = K(\dot q) - V(q) = \frac{1}{2}m\dot q^2 - \frac{1}{2}mq^2, \tag{5}$$

where q is the displacement from equilibrium. The damping is modeled as an external force $F(q,\dot q) = -\alpha m\dot q$.

For the discretization we use a linear-order discrete Lagrangian, and a corresponding linear-order quadrature for the external force $F(q,\dot q)$,

$$F^-_d(q_j,q_{j+1}) = hF\left(q_j, \frac{q_{j+1}-q_j}{h}\right) \qquad \text{and} \qquad F^+_d(q_j,q_{j+1}) = 0. \tag{6}$$

Therefore, the forced discrete Euler-Lagrange equations using a position-momentum formulation are

$$p_j = \frac{p_{j-1} - hq_{j-1}}{1+\alpha} \qquad \text{and} \qquad q_j = q_{j-1} + hp_j. \tag{7}$$

The modified Lagrangian and force for this system, being solved by a first-order forced discrete Euler-Lagrange equations are, respectively,

$$L_{mod}(q,\dot q) = L(q,\dot q) + h\frac{1}{2}\dot q\ddot q + \mathcal{O}(h^2) \qquad \text{and} \qquad F_{mod}(q,\dot q) = F(q,\dot q) - h\frac{1}{2}\alpha\ddot q + \mathcal{O}(h^2). \tag{8}$$

Herglotz' description: In this context the Lagrangian describing the system is

$$L(q,\dot q,z) = K(\dot q) - V(q) - \alpha z = \frac{1}{2}m\dot q^2 - \frac{1}{2}mq^2 - \alpha z. \tag{9}$$

The position-momentum formulation of the discrete Herglotz equations (3) are

$$q_j = \left(1 - \frac{h^2}{2}\right)q_{j-1} + h(1-h\alpha)p_{j-1} \qquad \text{and} \qquad p_j = (1-h\alpha)p_{j-1} - \frac{h}{2}(q_j + q_{j-1}). \tag{10}$$

As shown in [9], the modified Lagrangian for this system, being solved by a first-order contact integrator is

$$L_{mod}(q,\dot{q},z) = L(q,\dot{q},z) + h\frac{\alpha}{2}\left(\frac{1}{2}\dot{q}^2 - \frac{1}{2}q^2 - \alpha z\right) + \mathcal{O}(h^2). \tag{11}$$

We compare the qualitative behavior and the relative error of integrators (7) and (10). The reference solution is obtained using a Leapfrog method with a step size ten times smaller than the compared integrators. The code used is an extension of the code used in [9], in which we add our implementation of LA integrator. The results of the comparisons are shown in in Figure 1, in which we test the integrators using two damping parameters α. In both cases the Contact integrator shows a good qualitative behavior and much less relative error than the integrator based on LA principle.

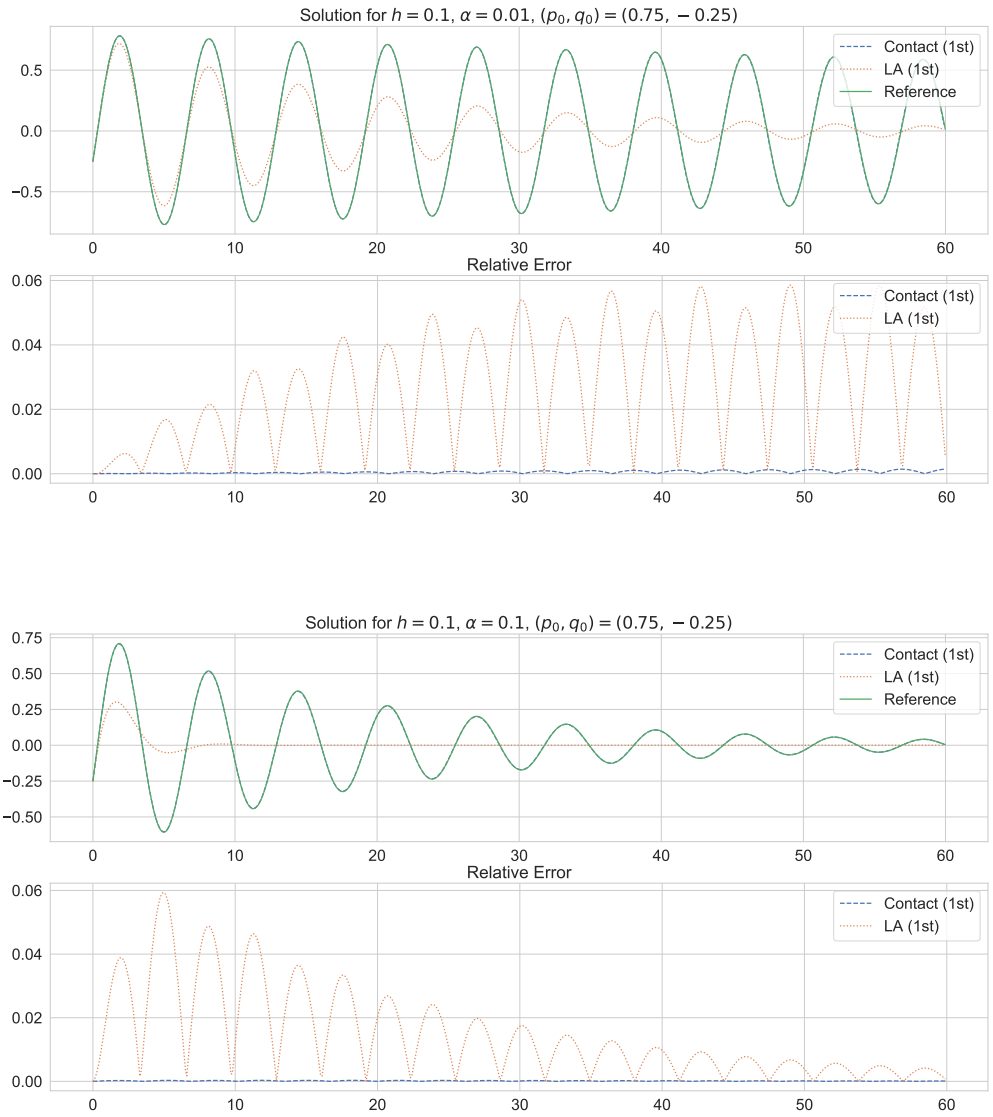

Figure 1. Damped harmonic oscillator simulation with a small damping parameter α using the Contact integrator and the integrator based on LA principle. In the Solutions, the x axis represents the time in seconds and the y axis represents the displacement from equilibrium of the oscillator, h is the time step and (p_0, q_0) represent the initial momentum and position, respectively.

3.2 Foucault pendulum

General setting and simplifications: The Foucault pendulum consists of a pendulum of length l and mass m located at latitude β on Earth's surface. We may consider here a Rayleigh dissipation with parameter α. The plane of oscillation does not rotate in a reference (X, Y, Z) fixed in space, hence as Earth rotates this plane rotates with respect to a reference (x, y, z) attached to Earth. To model this problem we consider the inertial frame (X, Y, Z) with origin at the center of the Earth, and Z passing through the north pole, hence, the angular velocity of Earth, Ω points along Z. On the other hand, the noninertial frame (x, y, z) is such that x points along a meridian in the south direction, y points to the east along the parallel β and z coincides with the vertical at the pendulum location. Hence, the vector position $r = (x, y, z)$ of a particle in the noninertial frame satisfies the relation $\omega = \frac{r\times\dot{r}}{\|r\|^2}$, where $\omega = (\Omega\cos\beta, 0, -\Omega\sin\beta)$ is the angular velocity of the particle in the noninertial frame.

As the pendulum forms a small angle ϕ in its oscillatory motion, the coordinates x, y are of order $l\phi$, whereas z is of order $l\phi^2$ and so it is negligible. Thus, we may consider the movement of the mass pendulum in the plane $z = 0$ and take $q = (x, y)$ as generalized coordinates. With these considerations, the kinetic energy $K(\dot{q})$ and potential energy $V(q)$, in terms of the mass m, the length l and the gravitational acceleration g, are given by:

$$K(\dot{q}) = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2) \qquad \text{and} \qquad V(q) = \frac{1}{2}m\frac{g}{l}(x^2 + y^2), \tag{12}$$

while the relation $\omega = \frac{r\times\dot{r}}{\|r\|^2}$ reads

$$-y\dot{x} + x\dot{y} + \Omega\sin\beta(x^2 + y^2) = 0, \tag{13}$$

which is a nonholonomic constraint for the system.

Lagrange-d'Alembert description: In this context, the Lagrangian is $L(q, \dot{q}) = K(\dot{q}) - V(q)$, which according to our previous computations reads

$$L(q, \dot{q}) = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2) - \frac{1}{2}m\frac{g}{l}(x^2 + y^2), \tag{14}$$

subject to the constraint (13). The damping is modeled as an external force $F(q, \dot{q}) = -\alpha m\dot{q}$.

To derive the integrator for this case we use equation (1) with a linear-order quadrature for both the Lagrangian and the external force, while the discrete constraint is obtained using the discretizing map Ψ on equation (13) (see [11]). The resulting equations are

$$\begin{aligned}
\frac{-x_{j+1} + 2x_j - x_{j-1}}{h} - h\frac{g}{l}x_j - \alpha(x_{j+1} - x_j) + \lambda_1\frac{y_j}{m} &= 0\\
\frac{-y_{j+1} + 2y_j - y_{j-1}}{h} - h\frac{g}{l}y_j - \alpha(y_{j+1} - y_j) - \lambda_1\frac{x_j}{m} &= 0\\
-y_j\frac{x_{j+1} - x_j}{h} + x_j\frac{y_{j+1} - y_j}{h} + \Omega\sin\beta(x_j^2 + y_j^2) &= 0,
\end{aligned} \tag{15}$$

where λ_1 is a Lagrange multiplier.

Herglotz' description: Here, the Lagrangian is taken as $L(q, \dot{q}, z) = K(\dot{q}) - V(q) - \alpha z$, which, according to our previous analysis becomes

$$L(q, \dot{q}, z) = \frac{m}{2}(\dot{x}^2 + \dot{y}^2) - \frac{mg}{2l}\left(x^2 + y^2\right) - \alpha z, \tag{16}$$

also subject to the nonholonomic constraint (13).

To derive the Contact integrator for this system we use a linear-order approximation in equations (4), i. e.

$$z_{j+1} - z_j = hL(x_j, x_{j+1}, z_j, z_{j+1}), \tag{17}$$

and the constraints are discretized in the same way as in [11]. The resulting equations are

$$\begin{aligned}
\frac{-x_{j+1} + 2x_j - x_{j-1}}{h^2} - \frac{g}{l}x_j - \alpha\left(\frac{x_j - x_{j-1}}{h} - \frac{h}{2}\frac{g}{l}x_j\right) + \lambda_1\frac{y_j}{m} &= 0\\
\frac{-y_{j+1} + 2y_j - y_{j-1}}{h^2} - \frac{g}{l}y_j - \alpha\left(\frac{y_j - y_{j-1}}{h} - \frac{h}{2}\frac{g}{l}y_j\right) - \lambda_1\frac{x_j}{m} &= 0\\
-y_j\frac{x_{j+1} - x_j}{h} + x_j\frac{y_{j+1} - y_j}{h} + \Omega\sin\beta(x_j^2 + y_j^2) &= 0,
\end{aligned} \tag{18}$$

where λ_1 is a Lagrange multiplier.

As can be noted, the discretization of the constraints in both integrators LA and Contact are the same.

The results of the comparisons are show in Figure 2, in which we test the integrators using two damping parameters α, for a Foucault pendulum of $m = 28$ kg, $l = 67$ m, latitude $\beta = 49°$ and step size $h = 0.1$, swinging for a time of 3600 s. In the first case, the dissipation is $\alpha = 0.001$ and both integrators show indistinguishable behavior in terms of energy dissipation and trajectory of pendulum bob. To model a more realistic pendulum with drag we decrease the value of the dissipation parameter to $\alpha = 0.0001$ for a second simulation, in this case the LA integrator displays an anomaly, as the energy of the system spuriously drops and the plane of oscillation changes direction in a discontinuous way at a given moment, whereas the Contact integrator, with the same parameters, does not suffer from these anomalies, displaying good qualitative behavior.

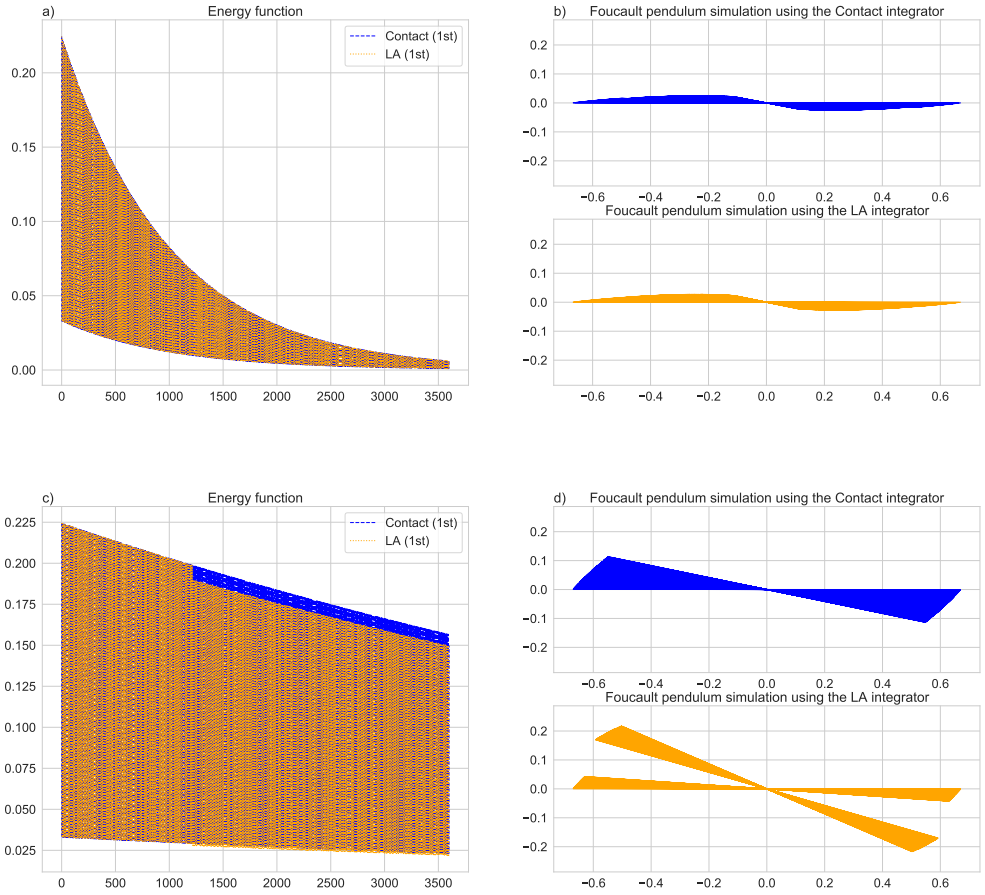

Figure 2. Foucault pendulum simulation with two values of the damping parameter α using the Contact integrator (blue) and the integrator based on LA principle (orange). In the plots a) and b), $\alpha = 0.001$, whereas in the plots c) and d), $\alpha = 0.0001$. In plot a) and c) are plotted the energy functions of the integrated systems and in the plots b) and d) are plotted the trajectories of the pendulum bob as simulated by the two integrators. In all the experiments the initial conditions are $q(0) = (0.67, 0)$ and $\dot{q}(0) = (0, 0)$.

4 Conclusions

In this paper, we construct a contact variational integrator incorporating nonholonomic constraints to an integrator coming from a discretization of Herglotz' principle.

With a numerical simulation of the damped harmonic oscillator (holonomically constrained), we demonstrate that this integrator outperforms the one coming from the Lagrange-d'Alembert principle (which displays overdamping). This is expected, since Herglotz' principle naturally incorporates the nonconservative nature of dissipative systems, while Lagrange-d'Alembert does not.

On the other hand, for the dissipative nonholonomic case, we perform numerical simulations of the damped

Foucault pendulum, and discover that the new integrator displays a good qualitative behavior, while the Lagrange-d'Alembert integrator (under the same conditions) presents qualitative anomalies. It is worth noting that one of the main interest behind variational integration is precisely the good qualitative behavior in long-time simulations. We want conservative systems to preserve their conserved quantities, we want continuous systems to display continuity, and so on. That being said, the anomalies displayed by the Lagrange-d'Alembert integrator disappear when we refine the time-step by a factor of 20, which certainly implies a computational cost that might be undesirable. A fundamental question raised at this point is the following: as it was already mentioned, the dissipative nature of systems are naturally incorporated into the Herglotz principle, and behind this is the fact that both Herglotz' principle and the dynamics of dissipative systems naturally fit into the framework of contact geometry. The situation regarding nonholonomicity is not so clear, and thus, it is unclear if the anomalous behavior of the Lagrange-d'Alembert is geometric in nature or it is purely a numerical issue.

The authors are enthusiastic with the numerical results obtained by this new integrator. At the moment, we are working in the backward error analysis of the variational integrators with nonholonomic constraints. This is an important issue, since it allows a quantitative way for comparing different models, and in some cases, it determines what kind of modifications can be implemented to construct better integrators as was illustrated in [14] for the holonomic situation.

Acknowledgements. The authors acknowledge the support given by FEEI-CONACYT-PROCIENCIA and the project POSG17-62-PROCIENCIA-CONACYT.

Authorship statement. The authors hereby confirm that they are the sole liable persons responsible for the authorship of this work, and that all material that has been herein included as part of the present paper is either the property (and authorship) of the authors, or has the permission of the owners to be included here.

References

[1] Hairer, E., Lubich, C., & Wanner, G., 2006. *Geometric numerical integration: structure-preserving algorithms for ordinary differential equations*, volume 31. Springer Science & Business Media.
[2] Marsden, J. E. & West, M., 2001. Discrete mechanics and variational integrators. *Acta Numerica*, vol. 10, pp. 357–514.
[3] Lanczos, C., 2012. *The variational principles of mechanics*. Courier Corporation.
[4] Lewis, A., 2003. Lagrangian mechanics, dynamics and control. *Preprint available*, vol. 237.
[5] de León, M., Jiménez, V. M., & Valcázar, M. L., 2019. Contact hamiltonian systems with nonholonomic constraints. *arXiv preprint arXiv:1911.05409*.
[6] de León, M. & Lainz Valcázar, M., 2019. Contact hamiltonian systems. *Journal of Mathematical Physics*, vol. 60, n. 10, pp. 102902.
[7] Bravetti, A., Cruz, H., & Tapias, D., 2017. Contact hamiltonian mechanics. *Annals of Physics*, vol. 376, pp. 17–39.
[8] Bravetti, A., 2017. Contact hamiltonian dynamics: the concept and its use. *Entropy*, vol. 19, n. 10, pp. 535.
[9] Vermeeren, M., Bravetti, A., & Seri, M., 2019. Contact variational integrators. *Journal of Physics A: Mathematical and Theoretical*, vol. 52, n. 44, pp. 445206.
[10] Bloch, A., Marsden, J. E., Crouch, P. E., & Baillieul, J., 2015. *Nonholonomic Mechanics and Control*. Springer.
[11] Cortés, J. & Martínez, S., 2001. Non-holonomic integrators. *Nonlinearity*, vol. 14, n. 5, pp. 1365.
[12] Modin, K. & Verdier, O., 2017. What makes nonholonomic integrators work? *arXiv preprint arXiv:1707.04514*.
[13] Vermeeren, M., 2017. Modified equations for variational integrators. *Numerische Mathematik*, vol. 137, n. 4, pp. 1001–1037.
[14] De La Torre, G. & Murphey, T., 2017. Surrogate lagrangians for variational integrators: High order convergence with low order schemes. *arXiv preprint arXiv:1709.03883*.