# An extension of the SHAKE and RATTLE methods for nonholonomic mechanics


Sebastián J. Ferraro*,†, David Iglesias‡ and David Martín de Diego‡

†Universidad Nacional del Sur, Bahía Blanca, Argentina; ‡ICMAT (CSIC-UAM-UCM-UC3M), Madrid, Spain.

*Presenting author — Email addresses: sferraro@uns.edu.ar – iglesias@imaff.cfmac.csic.es – d.martin@imaff.cfmac.csic.es


## 1 General setting

Nonholonomic mechanical systems where the Lagrangian is $L(v_q) = \frac{1}{2}g(v_q, v_q) - V(q)$, $v_q \in T_qQ$. Here $g$ is a Riemannian metric on $Q$. The discrete Lagrangian $L_d\colon Q \times Q \to \mathbb{R}$ approximates $L\colon TQ \to \mathbb{R}$.

Constraints linear in the velocities are given by a distribution $\mathcal{D} \subset TQ$. Complementary projectors: $\mathcal{P}\colon TQ \to \mathcal{D}$, $\mathcal{Q}\colon TQ \to \mathcal{D}^\perp$.

## 2 A geometric nonholonomic integrator

Discrete Euler–Lagrange equations (for *unconstrained* systems)

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

The proposed ***discrete nonholonomic equations*** are

$$\begin{aligned}\mathcal{P}^*_{|q_k}(D_1L_d(q_k, q_{k+1})) + \mathcal{P}^*_{|q_k}(D_2L_d(q_{k-1}, q_k)) = 0\\ \mathcal{Q}^*_{|q_k}(D_1L_d(q_k, q_{k+1})) - \mathcal{Q}^*_{|q_k}(D_2L_d(q_{k-1}, q_k)) = 0.\end{aligned}$$

The first equation is the projection of the discrete Euler–Lagrange equations to the constraint distribution $\mathcal{D}$, while the second one can be interpreted as an elastic impact of the system against $\mathcal{D}$ (see [4]). The second equation represents a three-point discretization of the constraints.

This defines a unique discrete evolution operator if and only if $(D_{12}L_d)$ is a regular matrix.

Define the pre- and post-momenta, which are covectors at $q_k$:

$$\begin{aligned}p^+_{k-1,k} &= \mathbb{F}^+L_d(q_{k-1}, q_k) = (q_k, D_2L_d(q_{k-1}, q_k))\\ p^-_{k,k+1} &= \mathbb{F}^-L_d(q_k, q_{k+1}) = (q_k, -D_1L_d(q_k, q_{k+1})).\end{aligned}$$

$\mathbb{F}^\pm L_d$ are the discrete Legendre transformations associated to $L_d$.

## 3 Preservation properties of the method

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

$$\mathfrak{g}^q = \left\{\xi \in \mathfrak{g} \mid \xi_Q(q) \in \mathcal{D}_q\right\}.$$

The bundle over $Q$ whose fiber at $q$ is $\mathfrak{g}^q$ is denoted by $\mathfrak{g}^{\mathcal{D}}$.

Define the discrete nonholonomic momentum map $J^{\mathrm{nh}}_d\colon Q \times Q \to (\mathfrak{g}^{\mathcal{D}})^*$ as in [1] by

$$\begin{aligned}J^{\mathrm{nh}}_d(q_{k-1}, q_k)\colon \mathfrak{g}^{q_k} &\to \mathbb{R}\\ \xi &\mapsto \left\langle D_2L_d(q_{k-1}, q_k), \xi_Q(q_k)\right\rangle.\end{aligned}$$

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

A horizontal symmetry is an element $\xi \in \mathfrak{g}$ such that $\xi_Q(q) \in \mathcal{D}_q$ for all $q \in Q$.

If $L_d$ is $G$-invariant and $\xi$ is a horizontal symmetry, then the proposed nonholonomic integrator preserves $(J^{\mathrm{nh}}_d)_\xi$, the **discrete nonholonomic momentum map**.

Let the configuration manifold be a Lie group with a Lagrangian defined by a bi-invariant metric and with an arbitrary distribution $\mathcal{D}$, and take a discrete Lagrangian that is left-invariant. Then the proposed method is **energy-preserving**.

## 4 Nonholonomic SHAKE and RATTLE

On $Q = \mathbb{R}^n$, consider the Lagrangian $L(q, \dot{q}) = \frac{1}{2}\dot{q}^TM\dot{q} - V(q)$ with $M$ invertible, and the constraints $\mu(q)\dot{q} = 0$, where $\mu(q)$ is a $m \times n$ matrix with rank $\mu = m$.

Symmetric discretization:

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

Our method yields the equations

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

This is an extension to the SHAKE method proposed by [5] to the case of nonholonomic constraints. SHAKE for holonomic constraints $g(q) = 0$ is

$$\begin{aligned}q_{k+1} - 2q_k + q_{k-1} &= -h^2M^{-1}\left(V_q(q_k) + g'(q_k)^T\lambda_k\right)\\ 0 &= g(q_{k+1}).\end{aligned}$$

The SHAKE methods involve a three-term recursion, which can lead to an accumulation of round-off errors. A reformulation as one-step methods is desirable (RATTLE). Define the momenta:

$$\widetilde{p}_k = \frac{1}{2}\left(p^+_{k-1,k} + p^-_{k,k+1}\right) = M(q_{k+1} - q_{k-1})/2h$$

$$p_{k+1/2} = M(q_{k+1} - q_k)/h$$

Rewriting the equations we get

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

Replace the last equation by an additional step of the algorithm:

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

Note that $\widetilde{p}_k$ lies on the constraint submanifold. Thus, there is a natural constraint on initial conditions: $\mu(q_0)M^{-1}\widetilde{p}_0 = 0$.

This suggests initial conditions for an algorithm on $Q \times Q$:

$$\mathcal{M}_0 = \{(q_0, q_1) \in Q \times Q \mid \mathbb{F}^-L_d(q_0, q_1) \in (\mathcal{D}^\perp)^o\}.$$

This can be used to initialize the algorithm for general $Q$ and $L$.

## References


[1] J. Cortés and S. Martínez. Non-holonomic integrators. *Nonlinearity*, 14(5):1365–1392, 2001.

[2] Y. N. Fedorov and D. V. Zenkov. Discrete nonholonomic LL systems on Lie groups. *Nonlinearity*, 18(5):2211–2241, 2005.

[3] S. Ferraro, D. Iglesias, and D. Martín de Diego. Momentum and energy preserving integrators for nonholonomic dynamics. *Nonlinearity*, 21(8):1911–1928, 2008.

[4] A. Ibort, M. de León, E. A. Lacomba, J. C. Marrero, D. Martín de Diego, and P. Pitanga. Geometric formulation of Carnot's theorem. *J. Phys. A*, 34(8):1691–1712, 2001.

[5] J.-P. Ryckaert, G. Ciccotti, and H. J. C. Berendsen. Numerical integration of the cartesian equations of motion of a system with constraint: molecular dynamics of $n$-alkanes. *J. Comput. Physics*, 23:327–341, 1977.